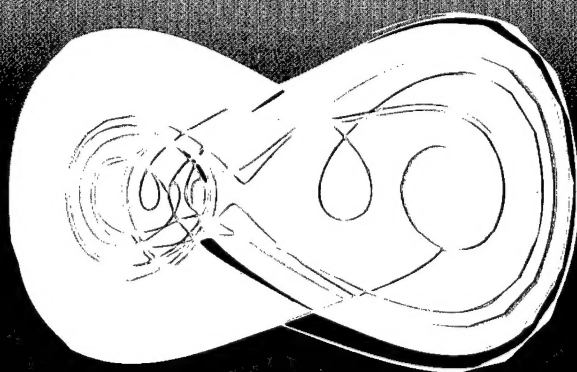


ARO 37280-1-RT-CF

8th
Brazilian Workshop on
SEMICONDUCTOR
PHYSICS



Águas de Lindóia / São Paulo - Brazil
February 2 - 7, 1997

PROGRAM and ABSTRACTS

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SOCIAL PROGRAM

Welcome Drink and Registration

All the participants and accompanying persons arriving on **Sunday, February 2**, are invited for a Welcome drink which will take place during the check-in at the hotel lobby, **from 16:00 on**. The registration desk will be opened for the participants to get registered from 14:00 to 20:00.

Opening Ceremony

The official opening of the BWSP-8 will be on **Sunday, February 2, 20:00, at the CAMERINO room**.

"Wednesday Night"

After dinner on **Wednesday, February 5**, there will be a performance of the *Quinteto de Cordas da Unicamp*. All the participants and accompanying persons are invited to enjoy the music.

SCIENTIFIC PROGRAM

Invited Speakers

Vladimir J. Trava-Airoldi (INPE, Brazil)
Israel Bar-Joseph (Weizmann Institute of Science, Israel)
Ayrton A. Bernussi (CPqD-Telebrás, Brazil)
Jarek Dabrowski (Institute for Semiconductor Physics, Germany)
Robert F. Davis (North Caroline State University, USA)
Vladimir Dmitriev (Howard Univerrsity, USA-IOFFE Institute, Russia)
Alexei L. Efros (University of Utah, USA)
Jochen Feldmann (Ludwig-Maximilians University Munich, Germany)
Jaime A. Freitas Jr. (Naval Research Laboratory, USA)
Jeffrey T. Glass (Kobe Steel USA Inc., USA)
Carlos F. O. Graeff (FFCLRP-USP, Brazil)
Pawel Hawrylak (Institute for Microstructural Sciences NRCC, Canada)
André B. Henriques (USP, Brazil)
Franz J. Himpsel (University of Wisconsin Madison, USA)
Hiroaki Inoue (Hitachi, Japan)
Thomas A. Kennedy (Naval Research Laboratory, USA)
M. Asif Khan (APA Optics Inc., USA)
Lionel C. Kimerling (MIT, USA)
Paul M. Koenraad (Eindhoven University of Technology, The Netherlands)
Klaus Lischka (University of Paderborn, Germany)
Eduardo R. Mucciolo (PUC-RJ, Brazil)
G. D. Pitt (Renishaw-University of Leeds, U. K.)
Flávio Plentz (UFMG, Brazil)
John Ryan (Oxford University, U.K.)
Werner Seifert (Lund University, Sweden)
Peter A. Schulz (UNICAMP, Brazil)
Michael G. Spencer (Howard University, USA)
Nelson Studart (UFSCar, Brazil)
Chris G. Van de Walle (XEROX, Palo Alto, USA)
Alex Zettl (University of California Berkeley, USA)

SCHEDULE	Mon 5/2	Tue 4/2	Wed 5/2	Thu 6/2	Fri 7/2
8:30-9:20	Zettl	Efros	Ryan	Davis	Himpel
9:20-10:10	Seifert	Bar-Joseph	Hawrylak	9:20-9:50 Freitas Jr. 9:50-10:20 Kennedy	Pentz
10:10-10:30	COFFEE-BREAK				
10:30-11:20	Stuart	Schulz	Mucciolo	10:40-11:10 Graeff 11:10-11:40 Spencer 11:40-12:10 Van de Walle	closing Koiller
11:20-12:10	Feldmann	Kimerling	Koenraad		
12:10-14:00	LUNCH				
14:00-14:50	Bernussi	Henriques		Lischka	
14:50-15:40	Inoue	Dabrowski		14:50-15:20 Glass 15:20-15:50 Khan	
15:40-16:00	COFFEE-BREAK				
16:00-18:30	POSTERS Session I	POSTERS Session II		16:10-16:40 Airoldi 16:40-17:10 Dmitriev 17:10-17:40 Pitt	
19:00-21:30	DINNER				
20:30-22:30	Round Table: Wide Band Gap Materials/Science and Technology				

MONDAY, FEBRUARY 3rd

Invited Talks Session 1

Chair: José R. Leite

- INV-01 8:30 **Alex Zettl:** *Novel Properties of Carbon and Non-Carbon Nanotubes.*
- INV-02 9:20 **Werner Seifert:** *Quantum Dots Grown In-Situ by MOVPE: Sizes, Densities and Optical Properties.*

Invited Talks Session 2

Chair: José R. Leite

- INV-03 10:30 **Nelson Studart:** *Theoretical Studies on Transport and Optical Properties of Delta-Doped Semiconductors.*
- INV-04 11:20 **Jochen Feldmann:** *Temporally and Spatially Resolved Optical Experiments on Semiconductor Quantum Wells and Quantum Dots.*

Invited Talks Session 3

Chair: Patrícia L. Souza

- INV-05 14:00 **Ayrton A. Bernussi:** *High Temperature Properties of Quaternary Quantum Well Laser Diodes.*
- INV-06 14:50 **Hiroaki Inoue:** *Semiconductor Optical Devices for Tera-bits/s Telecommunication Network.*

Poster Session I

Report to the Posters Program

TUESDAY, FEBRUARY 4th

Invited Talks Session 1

Chair: Maria J.S.P. Brasil

INV-07 8:30 **Alexei L. Efros:** *Insulator-Metal Transition in 2-d Interacting System.*

INV-08 9:20 **I. Bar-Joseph:** *Charged Excitons in GaAs Quantum Wells.*

Invited Talks Session 2

Chair: Maria J. S. P. Brasil

INV-09 10:30 **Peter A. Schulz:** *Electronic Structure of Lateral Superlattices: Hofstadter Spectra and Other Phenomena.*

INV-10 11:20 **Lionel C. Kimerling:** *Silicon for Photonics.*

Invited Talks Session 3

Chair: Marília J. Caldas

INV-11 14:00 **André B. Henriques:** *Magnetic Quantum Effects in Degenerate Superlattices.*

INV-12 14:50 **Jarek Dabrowski:** *Reconstruction Mechanisms of Silicon Surfaces.*

Poster Session II

Report to the Posters Program

WEDNESDAY, FEBRUARY 5th

Invited Talks Session 1

Chair: Enrique V. Anda

- INV-13 8:30 **John Ryan:** *Squeezed Light Generation in Semiconductors.*
- INV-14 9:20 **Pawel Hawrylak:** *Optical Probes of Elementary Excitations in Quantum Dots.*

Invited Talks Session 2

Chair: Enrique V. Anda

- INV-15 10:30 **Eduardo R. Mucciolo:** *Chaos and Universality in Mesoscopic Semiconductor Heterostructures.*
- INV-16 11:20 **Paul M. Koenraad:** *Correlated Dopant Distributions in Delta-Doped Layers Studied by Scanning Tunneling Microscopy and Magneto-Transport.*

THURSDAY, FEBRUARY 6th

Invited Talks Session 1

Chair: Jaime A. Freitas Jr.

- INV-17 8:30 **Robert F. Davis:** *Growth and Characterization of Bulk Crystals, Thin Films and Patterned Structures of AlN, GaN and Al_xGa_{1-x}N on SiC(0001) Substrates and Device-Related Research.*
- INV-18 9:20 **Jaime A. Freitas Jr.:** *Optical Studies of Undoped Wide Bandgap Carbide and Nitride Semiconductors.*
- INV-19 9:50 **Thomas A. Kennedy:** *Defects in ZnSe and GaN Studied with ODMR.*

Invited Talks Session 2

Chair: Jaime A. Freitas Jr.

- INV-20 10:40 **Carlos F.O. Graeff:** *Characterization of Polycrystalline Diamond Using Electron Spin Resonance.*
- INV-21 11:10 **Michael G. Spencer:** *AlN: A Versatile Wide Bandgap Material.*
- INV-22 11:40 **Chris G. Van de Walle:** *Defects and Doping in GaN.*

Invited Talks Session 3

Chair: Rolf Enderlein

- INV-23 14:00 **Klaus Lischka:** *Heteroepitaxy of Cubic GaN.*
- INV-24 14:50 **Jeffrey T. Glass:** *Diamond for Electronics.*
- INV-25 15:20 **M. Asif Khan:** *III-N Based Devices and Their Applications.*

Invited Talks Session 4

Chair: Rolf Enderlein

- INV-26 16:10 **Vladimir J. Trava-Airoldi:** *CVD-Diamond: An Overview on Research and Development at INPE.*
- INV-27 16:40 **Vladimir Dmitriev:** *Material Issues in High-Power Electronics on Wide Band Gap Semiconductors.*
- INV-28 17:10 **G. D. Pitt:** *Novel Raman Techniques for Spectroscopy, Imaging and Mapping in Wide and Narrow Gap Semiconductors.*

Round Table

- 20:30 **Wide Band Gap Materials/Science and Technology**
Chair: Robert F. Davis

FRIDAY, FEBRUARY 7th

Invited Talks Session 1

Chair: José A. Brum

INV-29 8:30 **Franz J. Himpsel:** *Semiconductor Research with Synchrotron Radiation.*

INV-30 9:20 **Flávio Plentz:** *Photoluminescence of a Two Dimensional Electron Gas in the Quantum Hall Effect Regime.*

Closing Session

10:30 **Belita Koiller**

POSTERS PROGRAM

Monday, February 3rd

Poster Session 1

• Bulk, Defects and Impurities

- MO-01 *Ab Initio Calculations of Carbon-Carbon Pairs in Silicon*
R.B. Capaz, A. Dal Pino Jr. and J.D. Joannopoulos
- MO-02 *Magneto-Optical and Magnetic Resonance Investigations of Intrinsic Defects in Electron Irradiated n-Type Al_xGa_{1-x}As*
M.V.B. Pinheiro, K.H. Wietzke, F.K. Koschnick, J.-M. Spaeth and K. Krambrock
- MO-03 *Ab Initio Electronic Structure Calculations of Zinc-Blende InN*
L.K. Teles, L.M.R. Scolfaro, R. Enderlein, J.R. Leite and J.L.A. Alves
- MO-04 *Study of the Diamond Crystal by Semiempirical Methods*
A.L.F. Marques and M.J. Caldas
- MO-05 *Ab Initio Study of Group V Elements in Amorphous Silicon and Germanium*
P.P.M. Venezuela and A. Fazzio
- MO-06 *Persistent Photoconductivity in p-Type Ge-Doped AlGaAs*
M.V.B. Pinheiro, K. Krambrock, A.S. Chaves, F.K. Koschnick and J.-M. Spaeth
- MO-07 *On the Stability of Fullerene-Like (BN)_n Clusters*
M.S.C. Mazzoni and H. Chacham
- MO-08 *First-Principles Calculation of Substitutional Oxygen and Oxygen-Hydrogen Complex in Gallium Arsenide*
W.M. Orellana and A.C. Ferraz
- MO-09 *Electrically Detected Spin-Dependent Recombination in Delta (Si) Doped GaAs Grown by MBE at Low Temperature*
K. Krambrock, M.V.B. Pinheiro, M.V.B. Moreira and A.G. de Oliveira
- MO-10 *Electronic Structure of Erbium-Oxygen Impurity Pairs in Silicon*
L.V.C. Assali and L.C. Kimerling
- MO-11 *Study of Conformational Defects on Organic Semiconductors: Polyacetylene and Polycarbonitrile*
J. del Nero and B. Laks
- MO-12 *Neutron Transmutation Doping of Silicon and Others Semiconductor Materials*
A.W. Carbonari and R.N. Saxena
- MO-13 *Defects Characterization of Irradiated Solar Cells Using Trigonometric Weight Functions*
P. Nubile
- MO-14 *Complex-Defects Related with Electrical Isolation by Ion-Irradiation in n-GaAs: A Theoretical Study*
A. Janotti, P. Piquini, R. Mota and A. Fazzio
- MO-15 *Multiphonon Assisted Transitions of Metastable Holes Generated by Strong Near Band Gap Light in GaAs*
W.V. Machado, E.C. Cipriano and M.A. Amato
- MO-16 *Electronic Structure of Point Defects in SiC*
H.W. Leite Alves

• Growth and Characterization

- MO-17 *On the Origin of Photoluminescence from InAs/InP Systems: The Competition Between 2D Structures and 3D Islands*
C.A.C. Mendonça, E. Laureto, M.A. Cotta, M.J.S.P. Brasil, M.M.G. Carvalho and E.A. Meneses
- MO-18 *Characterization of p-Type Si-Doped Semiconducting Structures Grown by Molecular Beam Epitaxy on (3,1,1)A GaAs Substrates*
M. Frizzarini, A.L. Sperandio, E.C.F. da Silva, A.A. Quivy and J.R. Leite
- MO-19 *Growth and Characterization of $\text{In}_x\text{Ga}_{1-x}\text{P}$ on GaAs by Chemical Beam Epitaxy*
J. Bettini, M.M.G. Carvalho, R. Yoshioka, J.W. Swart, C.A.C. Mendonça, M.A. Cotta and I.L. Torriani
- MO-20 *Utilization of a Four Layer Resist Process to Examine the Effects of Asymmetric Gate Recess on InGaAs/GaAs PHEMTs*
R. Grundbacher, D. Ballegeer, A.A. Ketterson, Y.-C. Kao and I. Adesida
- MO-21 *Adsorption and Dimer Exchange Process of As_2 Molecule over GaAs:Te, GaAs:Se and GaAs:S Surfaces*
R.H. Miwa and A.C. Ferraz
- MO-22 *Is There a Common Limiting Step in Diamond Growth Activation Energy?*
E.J. Corat, R.C.M. Barros, V.J. Trava-Airoldi, N.G. Ferreira, N.F. Leite and K. Iha
- MO-23 *Determination of Gas Phase Reactive Species in Chlorine Assisted Hot-Filament Chemical Vapor Deposition of Diamond by Mass Spectrometry*
R.C.M. Barros, E.J. Corat, V.J. Trava-Airoldi, N.G. Ferreira, N.F. Leite, V. Lemos and K. Iha
- MO-24 *Self-Assembled InAs Islands Morphology and Its Effect on the InP Buffer Layer*
I. Rasnik, M.J.S.P. Brasil, C.A.C. Mendonça, M.A. Cotta and M.M.G. Carvalho
- MO-25 *Mounds in GaAs Homoepitaxy: Formation and Evolution*
M.A. Cotta, V.R. Coluci, K.M. Ito-Landers, C.A.C. Mendonça and M.M.G. Carvalho
- MO-26 *Improvement of the Structural Properties of Near Stoichiometric PECVD SiO_2*
M.I. Alayo and I. Pereyra
- MO-27 *Kinetic Limit of Segregation During the Molecular Beam Epitaxy of GaAs/AlAs Heterostructures*
G. Zanelatto, Y.A. Pusep, D.I. Lubyshev, J.C. Galzerani and P. Basmaji
- MO-28 *The Carbon Incorporation in PECVD $\alpha\text{-Si}_{1-x}\text{C}_x\text{H}$ in the Low Power Density Regime*
I. Pereyra, M.N.P. Carreño, M.H. Tabacnicks, R.J. Prado and M.C.A. Fantini
- MO-29 *Differential Gain Analysis of InGaAs/InGaAsP/InP Multiquantum Well Lasers with 1.55 μm Emission Wavelength*
M.T. Furtado, W. Carvalho Jr., A.M. Machado and K. Jomori
- MO-30 *Secondary Ion Mass Spectrometry Analysis of Be Incorporation in InGaP*
M.A.A. Pudenzi, J. Bettini and M.M.G. Carvalho
- MO-31 *Growth of InGaAs Quantum Dots by Molecular Beam Epitaxy*
A.A. Quivy, A.S. Ferlauto and J.R. Leite
- MO-32 *Structural Characterization of Photoluminescence Porous Silicon with FTIR Spectroscopy*
W.J. Salcedo, F.J.R. Fernandez and E. Galeazzo
- MO-33 *Vertically Stacked Self-Assembled InGaAs Quantum Dot Layers Grown on (311)A/B and (001) Orientations*
P.P. González-Borrero, E. Petitprez, D.I. Lubyshev, E. Marega Jr. and P. Basmaji
- MO-34 *Intrinsic and Doped Microcrystalline Silicon Films for Application in Double Barrier Structures*
Z. Yu, M.N.P. Carreño, I. Pereyra, T.F. D'Addio and M.C.A. Fantini

- MO-35 *Effect of Thermal Annealing on a-Si_{1-x}C_x:H Deposited Under Silane Starving Plasma Regime*
C.A. Villacorta and I. Pereyra
- MO-36 *Growth of InAs Quantum Dots on GaAs Mediated by Te*
G.A.M. Sáfar, W.N. Rodrigues, M.V.B. Moreira, A.G. de Oliveira, J.M.C. Vilela, B.R.A. Neves, M.S. Andrade and J.A. Sluss
- MO-37 *Doping Efficiency in Highly Ordered PECVD a-Si_{1-x}C_x:H*
M.N.P. Carreño and I. Pereyra
- MO-38 *Very Low Hydrogen Content a-Si_{1-x}C_x:H Deposited Under Silane Starving Plasma Regime*
I. Pereyra, C.A. Villacorta and Z. Yu
- MO-39 *Natural Oxidation of Porous Silicon*
E. Galeazzo, A.E. Beltrán and F.J.R. Fernandez
- MO-40 *Filling Graphitic Nanotubes*
D. Ugarte, A. Chatelain and W.A. de Heer

• Optical Properties I

- MO-41 *Band Renormalization and Intervalley Scattering in Near Band Gap Femtosecond Optical Probing of AlGaAs Near the T'-X Crossover*
L.H.F. Andrade, P.A.M. Rodrigues, R. Marotti and C.H. Brito Cruz
- MO-42 *Optical Investigation of Interdiffusion in Narrow GaAs/AlAs Quantum Wells*
J.S. Michaelis, P.L. Souza and B. Yavich
- MO-43 *Micro-Raman Analysis of Minority Phase on Cubic/Hexagonal GaN Structures*
A. Tabata, R. Enderlein, P.K. Kiyohara, A.P. Lima, J.R. Leite, V. Lemos, D. Schikora, M. Kloidt and K. Lischka
- MO-44 *Optical Properties of Tetragonal HgI₂ and its Relationship with Crystalline Quality*
F.E.G. Guimarães, E.R. Manoel and A.C. Hernandez
- MO-45 *Inelastic Light Scattering Due to Coupled Plasmon-Phonon Modes in δ-Doped Semiconductors*
G.-Q. Hai, N. Studart and G.E. Marques
- MO-46 *Photoluminescence of Ge Islands Grown by Ultra High Vacuum-Chemical Vapour Deposition on Si (100)*
M. Cremona, F. Racedo, R. Larciprete and P.L. Souza
- MO-47 *Excitation Photoluminescence and Raman Scattering in Si-Planar Doped GaAs*
C.A. Siqueira and A.S. Chaves
- MO-48 *Photoreflectance and Time Resolved Photoreflectance in Delta Doped Superlattices (δ-Si:GaAs)*
M.J.V. Bell, D.F. de Sousa, L.A.O. Nunes and L. Ioriatti
- MO-49 *Optical Measurements of InAs Self-Assembled Quantum Dots Made by Surfactant Mediated Growth with Te*
G.A.M. Safar, W.N. Rodrigues, M.V.B. Moreira, A.G. Oliveira, S.L.S. Freire, L.A. Cury and H. Chacham
- MO-50 *Photoluminescence and Mobility of Single and Periodically Si δ-Doped InP Grown by LP-MOVPE*
B. Yavich, P.L. Souza, M. Pamplona-Pires, A.B. Henriques and L.C.D. Gonçalves
- MO-51 *Modulation-Doped Field-Effect Photodetectors*
M.A. Romero

- MO-52 *Photoluminescence Studies in Strained Si Single-Delta Doped InGaAs/GaAs Heterostructures*
A. Levine, E.C.F. da Silva, A.A. Quivy, J.A.N.T. Soares, V.A. Chitta and J.R. Leite
- MO-53 *New Results on Bound Excitons in Quantum Wells*
J.B.B. de Oliveira, E.A. Meneses and E.C.F. da Silva
- MO-54 *Spectroscopy of Optical Phonons in Strained GaSb/AlSb Superlattices*
S.W. da Silva, Y.A. Pusep, J.C. Galzerani, D.I. Lubyshev, A.G. Milekhin, V.V. Preobrazhenskii, M.A. Putiato and B.R. Semjagin
- MO-55 *Raman Analysis of Alloying Effects on Critical Layer Thickness in $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ Strained Heterostructures*
P.S. Pizani, J. Groenen, T.M. Boschi, F. Lanciotti Jr., R. Carles and M. Gendry

• Dots, Wires and Quantum Wells

- MO-56 *Electronic Structure of Holes in Modulation Doped $p\text{-Si}_{1-x}\text{Ge}_x/\text{Si}$ Strained Quantum Wells in a Magnetic Field*
L.G.C. Rego, P. Hawrylak and J.A. Brum
- MO-57 *Phase Diagram for Large Two Dimensional Bipolarons in a Magnetic Field*
W.B. da Costa and F.M. Peeters
- MO-58 *Depopulation of Electronic Subbands Induced by a Parallel Magnetic Field in an Asymmetrical Quantum Well*
A.R. Alves, P.S.S. Guimarães, L.A. Cury and M.V.B. Moreira
- MO-59 *Study of Magnetic Properties of Single-Electron Quantum Wires Systems*
P.J. von Ranke, R.B. Santiago and L.G. Guimarães
- MO-60 *Semiconductor Fibonacci Superlattices: Electronic and Optical Properties in the Presence of a Magnetic Field. Shallow Impurity States.*
A. Bruno-Alfonso, M. de Dios-Leyva and L.E. Oliveira
- MO-61 *Resonant Tunneling Used as an Optical Probe of Electron and Hole Dispersion Curves of a Quantum Well*
M.A.R. Souza and V.A. Chitta
- MO-62 *The Role of Graded Interfaces on the Acoustic Phonon Modes of Si/Ge Superlattices*
A.M.R. Teixeira, M.A. Araújo Silva, R.N. Costa Filho and V.N. Freire
- MO-63 *Impurity Excited States in GaAs Low Dimensional Systems Under Applied Electric Fields*
C.A. Duque and N. Porras-Montenegro
- MO-64 *Electronic Properties of V-Groove Quantum Wires Structures*
S.A. Leão and M.H. Degani
- MO-65 *Self-Consistent Hole Miniband Structure Calculations of Acceptor δ -Doping GaAs Superlattices*
L.E. Ramos, L.M.R. Scolfaro, G.M. Sipahi, R. Enderlein and J.R. Leite
- MO-66 *Electron and Hole States in Lead-Salt Semiconductor Heterostructures*
E.A. Andrada e Silva
- MO-67 *Energy Level Splitting in Doped Nonabrupt $\text{Al}_x\text{Ga}_{1-x}\text{As}$ Double Quantum Wells*
A.K. Freire, G.A. Farias and V.N. Freire
- MO-68 *Exchange Interaction of Disorder 2DEG on the Spin-Split Landau Levels*
I.G. Savel'ev, A.Y. Shik, G. Remenyi, G. Kovács, B. Pódör and G. Gombos
- MO-69 *Donor-Type δ -Doped Cubic GaN Superlattices and Quantum-Wells: Miniband Structure and Effective Masses*
S.C.P. Rodrigues, A.L. Rosa, L.M.R. Scolfaro, D. Beliaev, J.R. Leite, R. Enderlein and J.L.A. Alves

- MO-70 *Interface Form Birefringence in (311)A GaAs/AlGaAs Vertical Cavities with Native Oxide*
E.C. Valadares, L.A. Cury, F.M. Matinaga and M.V.B. Moreira

Tuesday, February 4th

Poster Session 2

• Transport Properties

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ABSTRACTS

INVITED TALKS

Novel Properties of Carbon and Non-Carbon Nanotubes

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Various form of nanotubes have been synthesized from carbon and other elements such a boron and nitrogen. I shall review the predicted and experimentally determined properties of these unusual structures, including structural, transport, and mechanical properties. The materials have intriguing conducting and semiconducting properties, including the possibility of on-tube electronic devices constituting only a handful of atoms, exceptionally high thermal conductivity, and elastic moduli exceeding those of any other insulating fiber.

**QUANTUM DOTS GROWN IN-SITU BY MOVPE:
SIZES, DENSITIES AND OPTICAL PROPERTIES**

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This talk focuses on the strain-induced self-organization, or "self-assembly" effect, producing quantum dots. Particularly the following aspects will be addressed: (i) the phenomenology of the 2D-3D morphology transition, (ii) the effects of materials choices and growth conditions on density, size and homogeneity of dots, (iii) manipulations to get laterally aligned and vertically stacked dot structures and (iv) optical properties of free-standing and buried dots of InP grown on GaInP/GaAs(001).

It will be shown that the control of the nucleation step for dot formation is the main tool to define the dot parameters. Nucleation determines the density of the dots, which increases with decreasing deposition temperature and increasing deposition rate. The size of the dots depends in first approximation on the available excess material per dot. For the same amount of deposition the sizes behave therefore inversely to the density. Increasing island size increases the strain-induced barrier around the coherent islands inhibiting the transport of material towards the island. Therefore, in contrast to "Ostwald ripening" (large islands grow on cost of smaller ones), the in-situ formation of dots narrows their size distribution.

Free-standing as well as buried dots of InP on GaInP/GaAs show luminescence and quantum confinement effects which depend on the size of the islands.

Luminescence arising from single dots will be demonstrated.

THEORETICAL STUDIES ON TRANSPORT AND OPTICAL PROPERTIES OF DELTA-DOPED SEMICONDUCTORS

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δ -doped semiconductors present a new important quasi-two-dimensional (2D) semiconductor system in which high electron density is attained and several subbands are occupied. A large number of experimental investigations have been carried out on the electron transport and optical properties in δ -layers. Novel and improved semiconductor devices have been fabricated from δ -doped structures. However, the theoretical studies on the electron transport and optical properties of δ -doped semiconductors are limited in some way. The present work is intended to present theoretical studies of the transport properties, many-body effects and optical properties of the δ -doped semiconductor systems. The paper emphasizes the following aspects:

1) The screening due to the 2D electron gas and of the ionized impurity scattering mechanism are analyzed for this multisubband system. We find that not only the intersubband scattering but also the intersubband coupling through the dielectric function in the screening plays an essential role in the ionized impurity scattering.

2) The subband quantum and transport mobilities are determined as a function of the doping concentration. The influence of the thickness of the doping layer and the background acceptor concentration are discussed. Furthermore, the calculation is extended to two coupled δ -layer systems.

3) The multisubband electron transport properties are studied for δ -layers which are subjected to an extra confinement coming from a quantum well (QW). We show that this extra confinement greatly enhances the intersubband interaction. At the onset of the occupation of a higher subband, the intersubband coupling leads to a reduction of the small angle scattering and, consequently, results in a significant increase of the quantum mobility.

4) The collective excitations and their coupling to optical phonons have been within the random-phase approximation. It is shown that, due to the high electron density in these systems in which several subbands are occupied, both intrasubband and intersubband plasmon modes are strongly coupled to the optical-phonon modes.

5) We obtain a very rich structure in the inelastic light scattering spectra due to charge-density and spin-density fluctuations. All the scattering peaks due to different intra- and intersubband modes can be observed. At small wave numbers, the peaks from the intersubband modes are the most pronounced, but the scattering from the intrasubband modes of the lowest subband is very strong at large wave numbers. However, due to level broadening effects, most of the scattering peaks are damped. Only a few main peaks remain with a large FWHM (full width at half maximum). Such a damping does not affect the phonon-like modes significantly and the scattering from these modes still can be clearly distinguished even with large broadening.

Temporally and spatially resolved optical experiments on semiconductor quantum wells and quantum dots

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Ultrafast laser spectroscopy has been used extensively to study carrier relaxation phenomena in semiconductor quantum wells. However, several important physical issues of electron-hole pair relaxation are still not understood satisfactorily. From an experimental point of view this is partly due to the fact that only electron-hole pair transitions with vanishing total wavevector ($K = 0$) can be optically excited and detected, provided no other quasi-particle carrying momentum is involved in the optical transition.

Here I report on temporally and spatially resolved optical pump and probe experiments performed on quantum wells to study the lateral diffusivity of excitons and electron-hole pairs as a function of time, excess energy, and crystal temperature. These measurements allow the investigation of the relaxation or cooling dynamics of excitons spread in K_{\parallel} -space.

In semiconductor quantum dots electrons and holes are confined in three dimensions leading to a density-of-states being a series of delta-functions. The above mentioned problem of how to optically measure carriers located in $K \neq 0$ states does not exist. Accordingly, solely time-resolved optical experiments are expected to monitor in detail the relaxation of electron-hole pairs in zero-dimensional semiconductor systems. I review our work on time-resolved photoluminescence experiments performed on stressor-induced InGaAs/GaAs quantum dots and discuss the roles of phonon- and Coulomb-scattering and of phase-space filling in the carrier relaxation scenario.

HIGH TEMPERATURE PROPERTIES OF QUATERNARY QUANTUM WELL LASER DIODES

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Quaternary quantum well laser diodes have attracted much attention in the last few years to their potential application to optical interconnects, fiber-in-the-loop and fiber-to-the-home systems. For these applications highly efficient cooler-free devices with low threshold currents and high slope efficiencies operating over the temperature range of -40°C to $+85^{\circ}\text{C}$ are desired. Multi-quantum well lasers (strained and lattice matched) with both quaternary InGaAsP wells and barriers have demonstrated to be very attractive sources capable of achieving the required performance. These devices exhibit reduced threshold current and high output characteristics at room temperature. However, the high-temperature properties of these devices have not improved as much as expected with the introduction of biaxial strain in the active region, despite the reduction of Auger recombination and intervalence band absorption. Hence, it becomes very important to clarify the physical mechanisms limiting the high temperature performance in these lasers. In this work we investigate the temperature sensitivity of $1.3\mu\text{m}$ multi-quantum well lasers with quaternary well and barrier materials, with different separate confinement heterostructure layer (SCH) thickness and internal biaxial strain values. Through a set of independent experiments such as spectrally resolved spontaneous emission, optical gain and differential carrier lifetime, and their respective temperature evolution, we identified the physical parameters limiting the high temperature performance of quaternary multi-quantum well lasers. The observed increase of carrier overflow into the barrier and SCH layers with injected current and temperature resulted in strongly increased internal losses contributing to a faster degradation of the slope efficiency at high temperatures. Carrier transfer processes, including finite capture time into the wells, carrier diffusion across the SCH layers and thermionic emission time, are the main physical mechanisms determining the increase of internal losses with temperature. Our results also suggest that the temperature dependence of differential gain and carrier density at transparency determines the temperature sensitivity of the threshold current in these devices.

SEMICONDUCTOR OPTICAL DEVICES FOR TERA-BIT/S TELECOMMUNICATION NETWORK

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Increasing demands for high-bit-rate transmission technologies enabling interactive multimedia era reach to establishing the global information infrastructure based upon optical tera-bit/s telecommunication network. The optical network, which fully utilizes optical bandwidth of fiber, will exploit the functionality offered not only by TDM (Time Division Multiplexing) but also by WDM (Wavelength Division Multiplexing) technologies. The optical high-bit-rate (TDM) and WDM transmission technologies accompanied by the optical node technologies such as WDM-ADM (Add/Drop Multiplexer) and WDM-OXC (Optical Crossconnect) require the even more functional optoelectronic devices. Semiconductor based optical devices is becoming more and more of a requirement as key devices, in terms of the advanced functionality, such as high-speed modulators over 10 Gb/s, compact optical amplifiers, matrix space switches, wavelength converters, and so on.

Here, we introduce our various types of semiconductor functional devices (GaAs and InP-based) for high speed modulators over 10 Gb/s (as TDM devices), gate switches with wavelength and polarization independence (as WDM devices), and routing switches (space switches) with lossless and compact features (as devices for optical node).

Especially, for high-speed devices, QCSE (Quantum Confined Stark Effect) in MQW (Multi-Quantum Well) is now going to play a major role in practical application. We introduce 10-40 Gb/s high speed MQW modulators for the forthcoming systems and ultra-small and up to 160 Gb/s modulators based on quantum confined polariton for future systems.

As for optical nodes and switching fabrics, space matrix switches are fundamental devices in order to fully utilize optical bandwidth. InP-based optical switches enable us to integrate optical amplifiers for large scale integration through loss compensation. And high speed gate switches for WDM signals would be also introduced for photonic switching devices.

A part of this work was carried out by the Quantum Functional Devices Project under the management of FED (the R&D Association for Future Electron Devices) as a part of the MITI (Japanese Ministry of International Trade and Industry) R&D of Industrial Science and Technology Frontier program supported by NEDO (New Energy and Industrial Technology Development Organization).

Insulator-Metal Transition in 2-d Interacting System.

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The question of an insulator-metal transition (IMT) in 2-d systems is very interesting and controversial. The one-particle scaling theory started by Abrahams *et al.* [1], now well established, predicts no IMT in 2d systems. Many-electron approach by Belitz and Kirkpatrick [2] predicts the same. However, the recent experimental data [3], obtained on Si-MOSFET structures, show that the transition does exist.

Theoretical study of the 2d correlated gas without magnetic field is based mainly upon the Hubbard and the t-J models (See review [4]). It is well known, however, that in the disordered system with localized electronic states the long-range part of the interaction is very important: the effects of the Coulomb interaction can not be considered as a perturbation at least at the vicinity of the chemical potential. The long range interaction provides the Coulomb gap in the one-particle density of states (ODS) in the localized regime. The ODS vanishes as energy tends to the chemical potential E_F . This fact disallows the Anderson-type scenario of the IMT with the delocalization of the states near E_F . This does not happen because such states do not overlap effectively. The elementary excitations, responsible for thermodynamics of the system, are the "soft pairs" of sites with a low energy of electron transition. At small hopping amplitude J these sites are resonant, and such pairs become the driving force of the IMT.

We consider the following Hamiltonian of the spinless fermions on a square lattice

$$H = \sum_i \varphi_i n_i + \frac{1}{2} \sum_{i \neq j} \frac{(n_i - \nu)(n_j - \nu)}{r_{ij}} + J \sum_{r,s} a_{r+s}^\dagger a_r \exp(i\mathbf{E}s). \quad (1)$$

External disorder is introduced by a set of random energies $-A < \varphi_i < A$, ν is the average filling factor. We consider a torus geometry with twisted boundary conditions. The ϕ -dependence of the total energy serves as a detector of delocalization [5]. All lengths are in units of a lattice constant, all energies are in units of n.n. Coulomb interaction.

We have performed a numerical diagonalization of the Hamiltonian Eq. (1) using truncated basis as proposed in Ref [6]. The filling factors are 1/2 and 1/4, $A = 0.5$, the total number of electrons is up to 32. The results can be formulated as follows:

1. Using different localization criteria including calculation of the Drude weight, we have found that transition from strongly localized to the diffusive regime occurs at $J < 0.1$ in the units of neighboring Coulomb interaction.
2. We have found that single-electron characteristics of the system including the spatial distribution of poles of the Green function and the ODS are much less sensitive to the change of J than many-electron characteristics under study.
3. The diffusion coefficient of electrons, as estimated from the Drude weight, is 10 times larger for interacting electrons than for non-interacting (cp. Berkovits *et al.* [7]).
4. We come to conclusion that the transition can not be described in terms of Anderson-type delocalization at the Fermi level. This is rather a "push me pull you" mechanism, where single-electron energies are not very important (cp. Shepelyansky *et al.* [8]).

We have also considered the 2d system of spinless fermions on a lattice without disorder ($A = 0$). At commensurate filling factors and at small J electrons form a Wigner crystal (WC) on a lattice. At filling factor $\nu = 1/6$ this structure melts at J as low as 0.02-0.03 in units of the nearest-neighbor Coulomb energy. We argue that this melting transition is connected to the dielectric-metal or dielectric-superconductor transitions.

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Charged Excitons in GaAs Quantum Wells

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The existence of charged excitons (trions) in semiconductors was proposed nearly 40 years ago: the negatively charged exciton (X^-), which consists of 2 electrons bound to a hole, and the positively charged exciton (X^+), which consists of 2 holes bound to an electron. These complexes are analogous to the well known hydrogen ions H^- and H_2^+ . The first observation of trions in two dimensional structures was only recently reported in CdTe/CdZnTe quantum wells (QW), where a spectral line associated with X^- was observed.

In this work we present our extensive study of trions in GaAs QW. By studying the shakeup luminescence lines associated with X^- we prove its three particle nature. We show that X^+ is formed in a two dimensional hole gas in an analogous way to the formation of X^- in a two dimensional electron gas (2DEG). We find that while the binding energy of the X^- and X^+ at zero magnetic fields are nearly the same, their evolution with magnetic field is very different. At high magnetic field we also observe the X_t^- , which is a negatively charged exciton with its two electrons forming a triplet state.

The system on which most observations of trions are made is a gated 2DEG. We observed a strong correlation between the changes in optical and transport properties with gate voltage. We shall show how these changes can help in better understanding the nature of the metal to insulator transition of this structure.

**Electronic structure of lateral superlattices:
Hofstadter spectra and other phenomena**

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Semiconductor nanostructures technology renewed the interest in a problem proposed at the beginnings of Quantum Mechanics: an electron in a periodic potential in the presence of a magnetic field. The electronic spectrum of this system shows interesting self-similar properties, ingeniously displayed twenty years ago in a "Hofstadter butterfly" representation. More recently, the ability to choose the lattice parameter of artificial two dimensional crystals, the so called lateral superlattices, brought the predictions of the existence of these self-similar spectra to accessible ranges of experimental conditions. However, we are dealing now with mesoscopic systems, defining a new complexity to the problem involving transitions from quantum to classical regime. Starting this journey from the extreme quantum limit, we discuss in this lecture general characteristics of the electronic structure of lateral superlattices, as well as the behaviour of the self-similar properties of these spectra as a function of the periodic potential modulation strength. Having in mind real systems, effects of the "crystal surface" will be briefly addressed. Yet an open problem, the observability of Hofstadter butterflies can be discussed with the elements given here. Finally, links between quantum and semiclassical regimes are suggested.

SILICON FOR PHOTONICS

INV-10

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The indirect gap of silicon leads to inefficient intrinsic luminescence, because three particles (electron, hole, phonon) must be involved. Localized impurity states provide efficient paths for e^-h^+ recombination by coupling to a source of local phonons for energy dissipation by nonradiative processes. Erbium, a rare earth ion, is an efficient recombination center and an efficient luminescent center. This unique circumstance arises because recombination involves the valence shell electrons of Si:Er, and light emission involves only the core-like, 4f shell electrons. Recombination energy is coupled into the 4f shell by an Auger-like process. The narrow emission spectrum at $\lambda = 1.54 \mu\text{m}$ is typical of Er^{3+} in glass hosts. However, in silicon the Er is excited by minority carrier recombination, whereas in glass hosts the Er is optically pumped. The relative excitation efficiency is approximately the ratio of the electronic capture cross section ($\sigma_{n,p} \sim 10^{-14} \text{ cm}^2$) to the optical capture cross section ($\sigma_p \sim 10^{-20} \text{ cm}^2$). Thus, electroluminescence in silicon has a $\times 10^6$ higher excitation efficiency than photoluminescence in Er-doped glasses.

The sharp line luminescence at $\lambda = 1.54 \mu\text{m}$ arises from the discrete $^4I_{13/2} \rightarrow ^4I_{15/2}$ transition from the excited, inner $4f^{11}$ shell of the Er^{3+} configuration. The energy balance between the recombination energy of electron-hole pairs and the excitation energy of f-electrons requires that excess energy be transferred to the free electron or defect vibration system. The excitation probability due to impact processes is proportional to the number of electrons with a kinetic energy larger than the $\sim 0.8 \text{ eV}$ excitation energy for Er^{3+} ions. Therefore, impact excitation can be an effective process for pumping Er-luminescence only in high electric fields.

High internal quantum efficiencies are only observed when the Er is surrounded by a strongly electronegative ligand field. The ligand field plays five critical roles in the optical activity of Si:Er: 1) The Er^{3+} -X center provides dipole coupling to channel e^-h^+ recombination energy into the 4f manifold. 2) The electronegative ligands strip charge away from Er and promote the formation of the optically active $4f^{11}$ configuration. 3) Local phonon modes of the ligands dissipate energy to promote resonant coupling of a portion of the recombination energy to the 4f manifold. 4) The ligand field adds to the silicon lattice contribution in breaking the inversion symmetry of the ion site. This symmetry breaking promotes admixing of states of opposite parity to allow the optical transition that is dipole forbidden for the isolated ion. 5) The ligand ions enhance the solubility of Er in silicon by the formation of localized complexes.

Erbium in Si with a high oxygen content shows a characteristic Si:Er-O photoluminescence spectrum with 5 lines due to the Stark splitting of the $4f^{11}$ ground state. With increasing annealing time the number of the oxygen related lines in the Er spectrum decreases. For a 60 hour anneal, discrete lines merge to an inhomogeneous broadening of the $1.54 \mu\text{m}$ emission line. This broadening is associated with the variety of local ligand structures. A direct correlation between Si:Er-O emission intensity and donor state introduction has been observed. The Er-O donor state energy position is $E_c - 0.16 \text{ eV}$. While this state has little overlap with the f-manifold wave functions, it acts as a gateway for energy flow to and from the Er f-shell.

LEDs emitting at room temperature have been fabricated by Er-O ion implantation. The devices show sharp line emission with a wavelength that is independent of temperature.

MAGNETIC QUANTUM EFFECTS IN DEGENERATE SUPERLATTICES

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The application of an intense magnetic field to semiconductor superlattices causes profound changes in the density of states of conduction electrons induced by the magnetic quantization of levels. For a magnetic field applied perpendicular to the epitaxial layers, the energy spectrum consists of a set of magnetic subbands separated by the cyclotron energy, and the density of states has singularities at the bottom and top of each magnetic subband. In degenerate systems, if the magnetic field is swept, the density of states at the Fermi energy has singularities each time a new subband crosses the Fermi level, which results in quasiperiodicity in $1/B$. This quasiperiodicity is reflected in an oscillatory behavior of the magnetoresistance (the Shubnikov-de Haas effect) and magnetophotoluminescence of these materials.

Recently a model for the magneto-oscillatory phenomena in degenerate semiconductor superlattices was elaborated in the frame of the tight-binding approximation and assuming a homogeneous Lorentzian broadening of the energy levels¹. The model explains the experimental finding of two magnetoresistance oscillatory components associated with each filled superlattice miniband in compositional superlattices (respective to the belly and neck orbits in k -space) and only the component due to the belly orbit in doping superlattices. Based on this theory Shubnikov-de Haas measurements made on InP with a periodical planar doping with silicon were interpreted to determine the miniband structure, wave functions and Fermi energy of charge carriers. The broadening of energy levels due to multiminiband scattering of carriers by ionized impurities was calculated using the random phase approximation (RPA), and it is in quantitative agreement with the energy level widths deduced from the Shubnikov-de Haas experiments. The latter calculations indicate that the electronic states belonging to the neck orbits have a lower quantum mobility than the belly ones, making their magneto-oscillatory contribution still less likely to be detected experimentally. Under tilted magnetic fields the magnetic breakdown effect is observed, whose signature provides a fine independent test of the theory. The photoluminescence of such systems in quantizing magnetic fields will also be presented and discussed.

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¹A.B.Henriques, Phys. Rev. B **50**, 8658 (1994)

Reconstruction Mechanisms of Silicon Surfaces

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We present an overview of reconstruction and chemisorption mechanisms on silicon. Si surfaces are the launching platform for microelectronics. Structural investigations of these surfaces are approaching their 40th anniversary. Until recently, some of the pieces of information needed to solve the jigsaw puzzle of the surfaces on the (001) to (110) azimuth had been missing. Our recent studies of Si(113) have revealed the most intriguing of these missing pieces. Though some questions still remain open, one can now attempt a survey of the basic mechanisms which drive the reconstruction of the clean silicon surfaces and which control the initial stage of thin film growth.

We focus on the new physical aspects brought forward by our recent studies of clean and Sb covered Si(113). The main body of the data was gained by scanning tunneling microscopy measurements and by *ab initio* pseudopotential calculations. We discuss how these results complete the atomic-scale picture of the (001) to (110) azimuth.

Like the Si(001), Si(111), and Si(110) surfaces, Si(113) forms naturally when the crystal approaches equilibrium. This interesting surface may be viewed as the limiting case of steps on Si(001) or on Si(111). The characteristic feature of Si(113) is its tendency to build up tensile stress. This is an effect of an adatom-like rebonding reminiscent of the rebonding at B-type steps of Si(001). The tensile stress promotes the appearance of some unusual structures built on the basis of *interstitial* atoms. On the clean Si(113), self-interstitials elevate molecular Si pentamers with benzene-like bonds. Sb passivation of the surface destroys the pentamers, but it may force some Si or Sb atoms into other interstitial sites.

When compared with the behaviors of clean and Sb passivated Si(001), Si(111), and Si(110), the results for Si(113) demonstrate how the interplay between surface stress, chemical bond energies, dangling bond density, and charge transfer determines the atomic structures and the chemisorption mechanisms. We also note that the reconstructions of Si(113) could be understood only when the measured data were augmented by *ab initio* calculations. This illustrates the need for such combined experimental and theoretical approaches in modern surface science.

SQUEEZED LIGHT GENERATION IN SEMICONDUCTORS

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Although the classical coherent electromagnetic field has a well-defined amplitude (E) and phase (F), the quantized field has vacuum fluctuations or photon shot noise which limit the minimum indeterminacy. Fluctuations in the quadrature components X and Y , where $E = \sqrt{3DE0} \{X\cos(\omega t) + Y\sin(\omega t)\}$, obey the uncertainty relation $\Delta X \Delta Y = \hbar/4$. A minimum uncertainty (MU) state, for example a coherent state, which is generated in a laser operating well above threshold, has $\Delta X = \Delta Y = \sqrt{\hbar/2}$. Currently there is much interest in developing light sources in which the fluctuations are squeezed below the quantum limit: the precision of optical measurements can be enhanced using squeezed light, and there are important potential applications in nonlinear optics and optical communications. From a semiconductor physics viewpoint, it is important to investigate the fundamental material properties which produce squeezing, and the mechanisms which lead directly to squeezed light generation in emitters such as lasers and LEDs.

The intrinsic third-order nonlinear optical susceptibility $\chi^{(3)}$ of semiconductors gives rise to four-wave mixing (FWM) of optical beams. If vacuum modes are incident together with a laser pump beam, the FWM process gives rise to the annihilation of two pump photons at frequency ω , and the generation of sideband photons at $(\omega = \omega_1 \pm \omega_2)$, with the modes experiencing amplification or de-amplification depending on their phase relative to the pump. In the case of de-amplification, the phase fluctuations can be reduced below the quantum limit. The state produced is quadrature squeezed: it is a MU state, and the amplitude fluctuations are increased above the quantum limit. These new states of light are extremely fragile, and any loss process which randomly annihilates photons quickly destroys the squeezing. For this reason the pump laser must be tuned below half-gap, where one and two-photon absorption are forbidden, and the material is essentially transparent. We will describe experiments using femtosecond laser pulses in which substantial quadrature squeezing is generated in II-VI materials using $\chi^{(3)}$ and $\chi^{(3)}$ which give rise to self-phase and cross-phase modulation respectively [1-3].

Photon number squeezed light can also be generated directly in semiconductor emitters using a sub-shot-noise current source, and the degree of squeezing depends on the electron-to-photon quantum efficiency of the device. These states are not MU states, and phase fluctuations can be large. However, as carrier injection in a laser diode is usually regarded as a random process, which would randomise photon emission, the observation of squeezing suggests that an underlying mechanism must regulate injection. Theoretical models have proposed a mechanism similar to Coulomb blockade, albeit macroscopic as opposed to microscopic effect [4]. This raises the intriguing possibility of quantum optical phenomena arising directly from quantum transport properties, and consequently to photon statistics providing a novel insight into carrier dynamics in semiconductors.

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Optical probes of elementary excitations in quantum dots

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Many electronic and opto-electronic devices are based on either the two-dimensional electron gas (Field Effect Transistor) or semiconductor quantum wells (Quantum Well Lasers). I will describe a class of quantum dots which are a natural product of the reduction of the lateral dimension to the nanometer scale. The gated, etched, and self-assembled dots (SAD) are studied in order to understand the role of reduced dimension and fabrication on their electronic and optical properties. The quantum dots filled with electrons form the heart of a quantum single electron transistor (QSET) while a quantum dot laser (QDL) contains both electrons and holes. The properties of QSET and QDL are determined by appropriate one- and two-particle spectral functions, which in turn are determined by elementary charge and spin excitations. We use Hartree, Hartree-Fock, and exact diagonalization methods to study the elementary excitation of quantum dots. The results of calculations are compared with electronic Raman, far infrared, and photoluminescence experiments. The charge density excitations of deep-etched modulation doped quantum dots are studied using resonant electronic Raman scattering. The magnetic field evolution of the spectra and a comparison with Hartree calculations shows the formation of the electronic shell structure in modulation doped quantum dots. The calculated shell structure and electronic excitations of charged SADs with a small number of electrons are compared with far infrared measurements. The comparison shows clearly the role of electron-electron interactions and spin in these artificial atoms. The operation of the quantum dot laser requires the understanding of many electron-valence hole complexes. We have carried out exact diagonalization studies of the ground state and elementary excitations of SADs containing up to twenty excitons. A remarkable addition/subtraction spectrum of excitons in SAD is obtained and explained in terms of condensation of excitons into coherent many-exciton states due to "hidden symmetries". The emission spectrum is determined by excitations of the electron-hole droplet. The unusual emission spectrum is responsible for the operation of a quantum dot laser.

CHAOS AND UNIVERSALITY IN MESOSCOPIC SEMICONDUCTOR HETEROSTRUCTURES

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Abstract

In recent years, some types of semiconductor heterostructures known as quantum dots have been used to study quantum and classical aspects of the electronic dynamics. Very clean samples can be made, such that the mean free path is large enough for the electron motion to be ballistic. In this regime, the dynamics is strongly influenced by the geometry of the confining potential. It has been found that statistical fluctuations of conductance in these systems have a universal character when the electron dynamics is chaotic in the classical limit (short wavelengths). In this seminar, we will review the main aspects of this problem, emphasizing recent experimental and theoretical results. Important questions still unanswered will be discussed.

Correlated Dopant Distributions in Delta-Doped Layers Studied by Scanning Tunneling Microscopy and Magneto-Transport

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The transport properties of free carriers in delta-doped layers have been studied extensively in recent years. The carrier mobility in these layers is rather low due to the strong scattering interaction between the free carriers and the ionized dopant atoms. In this paper we will show that also mutual interactions between the ionized dopant atoms can be strong and influence the transport properties of the free carriers in these doped layers. The magneto-transport properties of our delta doped layers were studied in magnetic fields up to 20 T. The spatial distribution of the dopant atoms was obtained by using Cross-sectional Scanning Tunneling Microscopy (X-STM) which is capable to discern individual dopant atoms.

We observe both from magneto-transport and X-STM measurements that the diffusion of Si as well as Be dopant atoms out of the doping layer is enhanced at high doping concentrations. In the case of Be delta-doped layers this is explained by the strong mutual repulsion of the ionized dopant atoms. In the case of the Si delta-doped layers Ga-vacancies might be involved in the diffusion rate enhancement. By studying the radial distribution function we observe that Coulombic repulsion also leads to an in-plane ordering of the Be dopant atoms. This structuring or correlation in the dopant distribution must influence the scattering of free carriers.

In order to assess the influence of these correlations in the dopant distribution we firstly performed a theoretical analysis of the carrier mobility in uncorrelated Si delta-doped layers. A good agreement between theory and experiment is obtained only when the screening is calculated using the well-known Random-Phase Approximation. The influence of correlations in the dopant distribution can now be included via the structure factor which is obtained directly from the radial distribution function.

It is still debated whether Si doped AlGaAs must be described by either the d^+/DX or d^+/DX_0 multi-valence system. In multi-valence systems, correlations in the charge distribution, instead of the real space distributions as discussed above, are to be expected. In delta-doped AlGaAs the ratio of d^+ to either DX or DX_0 scattering centers can be varied by application of hydrostatic pressure. Correlations in the charge distribution due to mutual interaction between the charged centers must vary as well when hydrostatic pressure is applied. This makes delta doped AlGaAs a perfect material to study the influence of correlations in the dopant distribution. We have measured the electron mobility in delta doped AlGaAs structures and find that only the d^+/DX -model, with the inclusion of correlations in the charge distribution, correctly describes the experimental results.

GROWTH AND CHARACTERIZATION OF BULK CRYSTALS, THIN FILMS AND PATTERNED STRUCTURES OF AlN, GaN AND $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ON SiC(0001) SUBSTRATES AND DEVICE-RELATED RESEARCH

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Single crystals of AlN to 1 mm thickness were grown at 1950-2250°C on 10x10 mm² 6H-SiC substrates via sublimation-re-condensation. Most crystals were 0.3mm - 1mm thick transparent layers completely covering the substrates. Raman, optical and TEM results will be presented. Single crystals of GaN were grown by subliming powders of this material under NH₃. Raman and photoluminescence results will be shown.

Monocrystalline thin films and heterojunctions of GaN and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys ($0.05 \leq x \leq 0.96$) were grown via OMVPE on 6H-SiC(0001) substrates at 1050-1100°C with (GaN) or without (alloys) an ≈ 100 nm thick, monocrystalline AlN(0001) buffer layer pre-deposited at 1100°C. Cross-sectional TEM revealed threading dislocations ($b = 1/3[1210]$) having a density in films grown on the on-axis substrates of $10^6 - 10^8/\text{cm}^2$ or $\leq (10^2 - 10^3)/\text{cm}^2$ than for films deposited simultaneously on the vicinal substrates. Both materials were free of low-angle grain boundaries and associated oriented domains. Biaxial strains resulting from mismatches in thermal expansion coefficients and lattice parameters in 22 GaN films, and measured via changes in the c-axis lattice parameter, were both tensile and compressive. Thus, the residual strain due to lattice mismatch was not completely relieved by defect formation. The PL spectra of the GaN films revealed strong bound excitonic emission with a FWHM value of 4 meV. Marked variations in the free excitonic emission and the c-axis lattice parameter with film stress were observed. A plot of near band-edge emission energy (determined by cathodoluminescence) vs. alloy composition revealed a negative bowing parameter. Controlled n-type, Si-doping in GaN was achieved for net carrier concentrations ranging from approximately $1 \times 10^{17} \text{ cm}^{-3}$ to $1 \times 10^{20} \text{ cm}^{-3}$. Magnesium-doped, p-type GaN was achieved with $n_A - n_D \approx 3 \times 10^{17} \text{ cm}^{-3}$, $\rho \approx 7 \Omega\text{-cm}$ and $\mu \approx 3 \text{ cm}^2/\text{V}\cdot\text{s}$. N-type (silicon) and p-type (magnesium) doping was achieved for $\text{Al}_x\text{Ga}_{1-x}\text{N}$ for $0.12 \leq x \leq 0.42$ and $x \leq 0.13$, respectively.

Selective growth of GaN and $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$ has been conducted on stripe and circular patterned GaN/AlN/6-H-SiC multilayer substrates. Growth morphologies on stripe patterns changed with their widths and the flow rate of TEG. Uniform hexagonal pyramid arrays of undoped GaN and Si-doped GaN were successfully grown on 5 μm circular patterns. Field emission measurements of a Si-doped GaN hexagonal pyramid array exhibited a turn-on field of 25 V/ μm for an emission current of 10.8 nA at an anode-to-sample distance of 27 μm .

Platinum-based ohmic and rectifying contacts have been fabricated via electron beam evaporation surfaces cleaned via Si deposition/flash evaporation techniques. Room temperature resistivities of the former were 1-10 $\text{ohm}\cdot\text{cm}$; however, they increased during annealing above 700°C as a result of significant chemical interdiffusion. The leakage currents of the latter contacts were 3-5 nA at -10V. The breakdown voltage was $\approx 40\text{V}/\text{cm}^2$. The results of additional electronic, device-related and device studies will also be reported.

Optical Studies of Undoped and Doped Wide Bandgap Carbide and Nitride Semiconductors

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The continuous progress in chemical vapor deposition techniques for homo and hetero-epitaxial growth of wide bandgap semiconductors has led to the successful fabrication and commercialization of an increasing number of devices using these materials. Full realization of the potential applications of wide bandgap ceramic semiconductors requires understanding the role of incorporation and activation of unintentional and intentional impurities, and structural defects. In this work a combination of defect-sensitive optical techniques have been used to study native defects and dopants in SiC and GaN.

Room temperature Raman scattering (RS) of SiC films deposited on Si-substrates indicate that the cubic phase of SiC crystallizes in the zinc-blend lattice with two atoms per unit cell. The low temperature photoluminescence (LTPL) spectrum of undoped films are characterized by a set of five sharp lines near 2.39 eV, and a set of broad lines and phonon replicas between 1.95 eV and 1.5 eV. The first has been assigned to a recombination process involving the annihilation of excitons bound to neutral nitrogen donors, and the latter to a recombination process associated with structural defects. PL studies of Al-doped films indicated that donor-acceptor pair (DAP) recombination process is the dominant recombination channel. Temperature studies of the DAP spectra infer a 54 meV binding energy for the nitrogen donor. The LTPL spectra of bulk cubic SiC are characterized by extremely sharp exciton lines and the absence of the deep defect band, commonly observed in hetero-epitaxial films. These observations verify the higher crystalline quality of bulk samples. High resolution PL measurements performed in the exciton spectral region shown the presence of lines associated with free-excitons, multiple excitons, multiple-phonon replicas of bound excitons, two-electron satellites, and lines associated with a shallower donor. FTIR experiments performed on the same samples confirm the 54 meV nitrogen binding energy value verified in the PL spectra in the two-electron satellite region. In addition, two others donors with lower concentrations with binding energies of 47.7 meV and 34 meV are observed.

Room temperature RS spectra of GaN films deposited on sapphire substrates show all six optical phonons expected for hexagonal GaN material. PL studies were carried out in undoped and doped GaN films grown by a low pressure metalorganic chemical vapor deposition technique in the temperature range between 6 K to 320 K. The PL spectra of undoped high resistivity films show well resolved spectral features which we have assigned to excitonic interband transitions. Analysis of the emission spectra of undoped high-resistivity, undoped high-conductivity and Si-doped films provide insights into the free-exciton binding energies and the binding energy of the excitons to neutral donors. Although Mg is the most commonly used p-type dopant for GaN, the activation of Mg-acceptors is still not well understood. Laser excitation intensity studies performed on Mg-doped samples show spectral shifts of the emission bands, which is typical for recombination processes involving DAPs. The largest difference in the emission spectra between undoped and Mg-doped films is the complete quenching of the 3.472 eV and 2.2 eV emission bands commonly observed in undoped films. In the Mg-doped film an intense band centered around 3.1 eV dominates the spectrum. This band is made up of a strong zero phonon line at 3.260 eV associated with distant donor-acceptor pairs and its LO-phonon replicas, separated by 92 meV. Upon increasing the concentration of activated Mg-impurities we observe changes of the line shape and peak position of the emission band attributed to recombination processes involving the Mg-acceptors and the residual donor. We will discuss different mechanisms which may be responsible for the observed behavior.

This work was performed in collaboration with W.J. Moore and was supported by the Office of Naval Research.

DEFECTS IN ZnSe AND GaN STUDIED WITH ODMR

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An overview of the current research on defects in ZnSe and GaN using Optically-Detected Magnetic Resonance (ODMR) is presented. The advantages and disadvantages of this technique for the study of defects in heteroepitaxial structures are outlined. The attempts to identify residual defects, to study the properties of n and p-dopants and to study defects which compensate the dopants are reviewed.

ODMR is a powerful technique for studying defects in heteroepitaxial systems. The method combines photoluminescence (PL) and electron paramagnetic resonance (EPR). Since it derives its sensitivity from PL, ODMR can detect defects in thin layers with concentrations of 10^{15} cm^{-3} or less. Conversely, since its resolution derives from EPR, it can resolve g-tensors and hyperfine interactions for the defects involved in recombination. Furthermore, ODMR provides correlated information on both the atomic and electronic structure of the defects involved. The effectiveness of ODMR can be limited by inhomogeneous strain and dislocations and by the complicated recombination processes which arise in heavily doped layers.

ZnSe grown on GaAs is under intense study because of its potential for optoelectronic applications. Most layers are 1-2 microns thick with uniform strain from thermal mismatch and a relatively low dislocation density. There is a large database on defects in bulk ZnSe in both the areas of PL and EPR. ODMR consisting of three resonances in N-doped ZnSe-GaAs was first reported by the group at Heriot-Watt University. One of these was assigned to effective-mass donors such as Cl or Ga. Subsequent work has shown that both the other resonances are also donors; one involving a Se-vacancy and the other probably related to the dislocations near the ZnSe/GaAs interface. Hence all three centers act to compensate the N-acceptor. Current work done in collaboration with Columbia and Florida Universities reveals another resonance which may be due to the N-acceptors themselves.

GaN grown on sapphire or SiC is also under intense study for optoelectronic and other applications. Most layers are 1-10 μm thick with some residual uniform strain from thermal mismatch but a large dislocation density. The data base for defects in GaN is small in both PL and magnetic resonance. EPR of the residual donor was first reported by Carlos and co-workers. ODMR of the 2.2 eV emission reveals signatures of two defects. One is clearly related to effective-mass donors and the other is assigned to a deep defect from its g-value and linewidth. Lack of hyperfine splitting has precluded a convincing identification so far. The Freiburg group initially reported the ODMR associated with Mg-doping and its compensating centers. The Mg-related state detected is not fully effective-mass-like. Both effective-mass and deep donors act to compensate the Mg. Current work at NRL has revealed resonances associated with the 3.0 eV emission seen in high-resistivity GaN.

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CHARACTERIZATION OF POLYCRYSTALLINE DIAMOND USING ELECTRON SPIN RESONANCE

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Electron spin resonance (ESR) and related techniques are shown to be useful and versatile in characterizing electronic as well as structural properties of polycrystalline diamond films. The observed ESR spectra of polycrystalline diamond films consisted basically of two contributions. A carbon vacancy-related signal with $g = 2.0028$ and width $\Delta H_{pp} \approx 4$ G, and a N-related signal with a central line at $g = 2.0024$ and $\Delta H_{pp} \approx 0.17$ G and hyperfine satellites. The second line is assigned to isolated substitutional nitrogen, the so called P1 center. The density of N-related paramagnetic states is strongly affected by illumination and heat treatment. Through systematic studies of these changes, using also other spectroscopic techniques such as photo-conductivity, it is found that the P1 center in CVD diamond gives rise to a deep donor state about 1.5 eV below the conduction band. The mechanism of nitrogen incorporation, and the consequences on the band gap density of states are discussed. The line-shape of the P1 center observed by ESR is found to be affected by crystallite disorientation. A simple model is proposed to introduce ESR as a quantitative method to characterize diamond films texture. The general conditions in which the method can be applied, and its applicability are discussed.

AlN: A VERSATILE WIDE BANDGAP MATERIAL

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In the last few years there has been a great deal of effort put into understanding the properties of a class of materials referred to as the "wide bandgap semiconductors". The principal materials in this grouping are SiC and GaN. The conventional wisdom asserts that SiC is the most likely material to produce a new generation of high power/high temperature devices, while GaN and related alloys show exciting promise as the foundation for opto-electronic devices in the visible and the ultraviolet. In this talk we would like to discuss the status and current problems in the development of another wide bandgap semiconductor material AlN. AlN is a wide bandgap semiconductor which has many interesting properties for high power applications (when used with SiC) as well as opto-electronic applications (when mixed with GaN or InN). One of the most important features of AlN is that the lattice constant of AlN and SiC forms the best lattice match system among the "widebandgap semiconductor" (.97%) binaries. Because of this favorable lattice match AlN is being considered for use as a gate dielectric for SiC transistors. In that role AlN is attractive because of its high temperature physical stability as well as its dielectric constant (8.4) which is significantly higher than SiO₂. AlN is currently used as a buffer layer in the growth of GaN on sapphire or SiC and is also used as a cladding material in In_{1-x}Ga_xN based laser structures. One property of AlN which is recognized but not yet fully exploited is piezoelectricity. Another application for AlN is optics where both the wave guiding and nonlinear optic properties of the material are interesting.

In our laboratory we have fabricated insulating and conducting films of AlN by the MOCVD technique. The insulating films have low oxygen and carbon content as measured by Auger spectroscopy. The best of these films show near band edge cathodoluminescence. Insulating films of AlN grown on 6H-SiC in the best of cases exhibit a step flow mode as seen by Atomic Force Microscopy (AFM). MIS capacitors fabricated with this material have exhibited very good electrical properties. Capacitance-voltage curves measured from these devices exhibited depletion, accumulation and evidence of inversion. Conducting films of AlN have been grown by heavy doping with carbon. These films exhibit a resistivity as low as 1 ohm-cm. In addition to basic electrical measurements some optical structures have been fabricated and measured. These optical structures include high speed Auston switches as well as optical waveguides. Using the optical waveguides we have made a careful determination of the refractive index of AlN.

DEFECTS AND DOPING IN GaN*

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GaN is successfully being used for green, blue, and UV light emitters and for high-temperature or high-power applications. The ability to control doping is crucial for device fabrication; wide-band-gap semiconductors such as GaN have long suffered from limitations on the achievable doping levels. *p*-type doping has become possible through a post-growth activation step, related to the presence of hydrogen in the material. The origin of the *n*-type conductivity in as-grown material has been debated until recently. I will discuss how theoretical results for native defects and dopant impurities, obtained with state-of-the-art first-principles calculations,¹ can be used to understand the various factors that limit doping. Specifically, I will show that the *n*-type conductivity can **not** be attributed to nitrogen vacancies, but is due to unintentional incorporation of donor impurities such as silicon or oxygen.² For *p*-type doping, we have investigated the incorporation of magnesium, the role of hydrogen,³ and the potential use of other acceptor impurities.⁴ I will also discuss the role of native defects in compensation and as recombination centers. Specifically, we propose that gallium vacancies are responsible for the "yellow luminescence".⁵

*Work performed in collaboration with Jörg Neugebauer and supported by DARPA.

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HETEROEPITAXY OF CUBIC GaN

INV-23

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In the last years, the wide bandgap semiconductor GaN has received increasing attention because of its applications for optoelectronic devices emitting light in the blue and ultraviolet spectral region. The polytype group III nitrides are naturally stable in the hexagonal (wurtzite) structure. However, successful epitaxial growth of metastable cubic phase GaN (c-GaN) has been accomplished by various groups in the past. Epitaxial grown layers of c-GaN lend themselves to the production of cleaved laser cavities. This is expected to be an interesting alternative to dry-edged cavities as already realized with hexagonal GaN based devices. In this paper, recent results of the molecular beam epitaxy (MBE) of c-GaN layers on GaAs (001) are reviewed.

It is firmly established that the growth of homogeneous c-GaN layers depends crucially on the control of the stoichiometry of the layer surface during growth. The importance of the observation of the surface reconstructions by reflection high energy electron diffraction (RHEED) and the establishment of a surface phase diagram is stressed. Self-consistent tight-binding total energy calculations are employed for theoretical modelling of the surface reconstruction and the results are compared to experimental data. The layers grown by MBE under nearly stoichiometric conditions are highly homogeneous and show negligible inclusions of wurtzite phase subdomains within the cubic lattice. This is demonstrated by Raman and micro-Raman experiments and by X-ray reciprocal space mapping. Hall effect measurements performed with undoped c-GaN layers reveal an extremely small density of residual impurities. Layers grown under slightly Ga or N-rich conditions show p and n-type conduction, respectively. The low-temperature photoluminescence spectra consist of well separated lines at 3.26 and 3.15 eV, which are identified to be due to excitonic and donor-acceptor pair transitions. No emission above the bandgap of the cubic phase is detected. Since photoluminescence is excited with an unfocused laser beam it is believed to resemble the layer properties rather than the properties of micron-size inclusions of micro-crystals. This result is corroborated by spatially resolved cathodoluminescence measurements which give the variation of the luminescence intensity with submicron resolution. The temperature-dependence of the photoluminescence lines reveal the binding energy of the donor and acceptor involved in the donor-acceptor pair recombination. The donor energy is 25 meV and the acceptor energy is about 130 meV, respectively. At room temperature an emission band at about 3.21 eV is observed with a full width at half maximum down to about 50 meV.

DIAMOND FOR ELECTRONICS

INV-24

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Diamond has fascinated scientists for many years due to its superb combination of unique properties, including: high thermal conductivity; optical clarity; hardness; high breakdown voltage, high Hall mobility; and negative electron affinity. It was not until the relatively recent discovery of chemical vapor deposition (CVD) that diamond generated wide spread interest in the electronics industry. CVD has allowed the deposition of thin films of diamond on various substrates making diamond compatible with electronic device fabrication. Doping of diamond has also been facilitated adding semiconductor qualities to a normally excellent insulator. Finally, the CVD technology also offers the promise of reduced cost for a variety of electronics-related applications.

This presentation will discuss the state-of-the-art of three major areas, if time allows: 1) deposition technologies; 2) diamond growth and electronic properties; and 3) electronic devices. A review of current deposition techniques most heavily used in industry will be given. This includes DC plasma jets, hot filament, and microwave plasma. Although numerous other systems are in use at various university and national labs, as well as some industrial R&D centers, none have found the widespread commercial application of these three primary techniques. DC plasma jet techniques tend to be utilized for high rate deposition of thick films for such applications as heat sinks. The advantages of the hot filament system involve rapid construction and low cost of the capital equipment for thin films applications in which film purity is not the highest priority. Microwave plasma systems offer the promise of large area deposition coupled with high film quality, particularly attractive for applications involving diamond on semiconductor wafers.

The growth and electronic properties of diamond will also be reviewed. Homoepitaxial, highly oriented, and random polycrystalline films have all been utilized for various applications. Several methods for achieving electronic diamond have been pursued and will be discussed. For example, bias enhanced nucleation has enabled highly oriented diamond growth. A multi-step thermal treatment has also shown promise for oriented diamond. Diamond is also being pursued by a "tiling" method. Hall mobilities exceeding those of typical boron doped natural diamond have been achieved through homoepitaxial CVD. Capacitance voltage measurements have verified differences in compensation for various films. Negative electron affinity has been measured in diamond through photo emission. Finally, photoconductivity results will be discussed.

With regard to devices, focus will be given to three classes of devices believed to be of most interest commercially: detectors; emission devices; and surface acoustic wave devices. Detectors include both particle detectors of interest for various types of high energy physics facilities and ultraviolet detectors for use in industrial applications. Collection distance and carrier lifetimes determine the performance of such devices. Emission devices include potential cold cathodes for various electron beam instruments in addition to flat panel displays and electron beam switches. Although diamond has been convincingly shown to yield negative electron affinity, field emission devices have not been able to take advantage of this property to date. Surface acoustic wave devices take advantage of diamond's high acoustic velocity. These devices are expected to enhance portable electronic devices, such as cellular phones, at high frequencies.

III-N BASED DEVICES AND THEIR APPLICATIONS

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Unique optical and electronic properties of the GaN/AlGa_N material system open up numerous opportunities for visible-blind optoelectronic devices. These devices have a high sensitivity and a large gain-bandwidth product and can be integrated with GaN/AlGa_N field effect transistors which have already demonstrated an operation at microwave frequencies. A transparent sapphire substrate also makes AlGa_N/GaN based devices uniquely suited for optoelectronic applications. We recently reported on GaN based optoelectronic devices, which included InGa_N-AlGa_N Light Emitting Diodes (LEDs), GaN photoconductive, Schottky barrier, and p-n junction ultraviolet detectors and optoelectronic AlGa_N-GaN Heterostructure Field Effect Transistors. In this paper, we review our recent results on InGa_N-AlGa_N Multiple Quantum Well Light Emitting Diodes on sapphire and spinel substrates and blue-green Mg-doped InGa_N-GaN Multiple Quantum Well Light Emitting Diodes, fabricated using low pressure metal-organic chemical vapor deposition. We also report on high responsivity, intrinsic photoconductors based on Al_xGa_{1-x}N with a long frequency cutoff from 350 to 240 nm.

A high peak velocity, high saturation velocity, and a respectable low field mobility of GaN indicate a good potential of the GaN based material system for microwave and millimeter wave applications. In this paper, we review our recent results on short channel GaN/AlGa_N Doped Channel Heterostructure Field Effect Transistors (DC-HFETs) with cutoff frequencies, f_T , above 36 GHz and maximum frequency of oscillation above 97 GHz and on one micron gate GaN/AlGa_N DC-HFETs, which exhibited f_T times gate length product comparable to that of GaAs MESFETs. In addition we will also discuss the recent results from other leading edge research and development groups.

**CVD-DIAMOND: AN OVERVIEW ON RESEARCH AND DEVELOPMENT AT
INPE**

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CVD diamond has achieved very important status in the world science and technology development after the beginning of the 80's. It has a unique set of superior properties and is long recognized to be the material of choice for many applications. At this time the CVD diamond, because of the challenge to explain the growth mechanism, the spreading of application areas and the simple synthesis processes, became an interesting area of investigation. Spatial technology area is optimistic about the real possibilities of improving the life time of some materials and by using CVD diamond in spacecraft as heat sinks, protective coating and tribological devices. At Instituto Nacional de Pesquisas Espaciais-INPE, besides space interest, we are expanding our contribution to some near and long term applications. In this work we present the state of the art of our research and development, as an emerging technology for many applications. Emphasis will be given on CVD diamond deposition mechanisms studies when halogenated gases are added to conventional mixtures. Also, investigations of the adherence and stresses between diamond films and several kinds of substrate materials like cemented carbide tools, quartz, and Ti6Al4V alloy will be presented. Finally, studies of columnar growth of free-standing films used for developing abrading surfaces including a scaling up for the initial production of a specific CVD diamond device are presented too.

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MATERIAL ISSUES IN HIGH-POWER ELECTRONICS ON WIDE BAND GAP SEMICONDUCTORS

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Wide band gap semiconductors, mainly SiC, have been considered as the materials for new generation of high-power electronic devices for a long time. It was predicted that due to high thermal conductivity and high electric breakdown field, SiC devices may have higher switching power than Si devices. Progress in SiC bulk and epitaxial growth technology made it possible to fabricate devices having predicted characteristics, particularly pn diodes blocking 4.5 kV², and thyristors³ operating at a forward current density of 1 kA/cm². However, the switching power in SiC devices does not exceed 10 kW and is much smaller than for comparable Si devices (> 1 MW). In this report, we discuss material issues limiting high-power performance of wide band gap semiconductor devices.

A principal factor limiting the forward current (≤ 10 A) in SiC devices is the small device area which is usually less than a few square millimeters. If a large die size is used, premature electric breakdown is observed. The nature of defects causing pre-mature electric breakdown for SiC devices with larger area is unknown. Possible candidates for the limiting defects are: 1) polytype micro-inclusions; 2) impurity clusters; 3) local inplanarity of the pn junction interface; 4) dislocations, and 5) micropipes.

Another problem with SiC devices is the high on-resistance. The factor responsible for high on resistance of high voltage SiC devices is a small minority carrier diffusion length (L_d). For SiC pn diodes and thyristors, the thickness of the base region of the device should be about 50 μm for 5 kV device and 100 μm for 10 kV device, respectively. Electrical conductivity of the base region material is low because of low carrier concentration in this region ($\leq 10^{15} \text{ cm}^{-3}$). To modulate the conductivity, the diffusion length of minority carriers should be at least 10 μm for 5 kV device and 20 μm for 10 kV device. The maximum L_d value measured so far for SiC pn structure is less than 2 μm . High resistivity of unmodulated part of the base region of the device will cause large forward voltage drops (up to 100 V). Possible ways to improve diffusion length (life time) in SiC pn structures will be discussed.

Recently, GaN pn junctions have been investigated and some fundamental parameters, such as electric breakdown field, temperature coefficient of breakdown voltage have been measured⁴. We will compare GaN and SiC properties and state of the art technology with respect of high-power device fabrication.

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Novel Raman Techniques for Spectroscopy, Imaging and Mapping in Wide and Narrow Gap Semiconductors

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A revolution has occurred in the past five years in Raman measurement techniques. Measurements are no longer difficult, owing to the use of specialised filters and cooled CCD detector arrays. Use of the single stage monochromator system incorporating notch filters will provide a throughput of $> 30\%$, compared with $< 1\%$ for traditional double or triple monochromators. The high optical throughput has given rise to the use of lower power (e.g. < 10 mW) lasers, and also greater system stability. With care, monolayer structures on silicon can be routinely examined, and strain maps, both laterally (resolution $< 1\text{ }\mu\text{m}$), and vertically (resolution $< 2\text{ }\mu\text{m}$) can be obtained in suitable semiconductor structures. A further extension of such systems has been the development of near field spectroscopy, giving spatial resolution below 100 nm .

Results will be presented for:

- a. Monolayers and near field microscopy on silicon.
- b. Strain mapping of device structures in silicon on 0.002% resolution.
- c. GaN Raman impurity mapping and imaging.
- d. Diamond Raman and photoluminescence combined measurement with strain and defect mapping using novel extended scan methods.
- e. Narrow gap In/GaSb alloy measurements.

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Semiconductor Research with Synchrotron Radiation

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Synchrotron radiation offers a variety of incisive techniques to map out semiconductor surfaces and devices. An overview of the current capabilities and future developments will be given.

A prominent asset of synchrotron radiation techniques is their surface sensitivity. Photoelectron spectroscopy and absorption spectroscopy of core levels detect surface species in etching and growth of semiconductors. They distinguish not only the stoichiometry, but also the local chemical bonding partners. For example, the various oxidation states of Si and B can easily be distinguished at the Si-SiO₂ interface and in BN thin films. X-ray diffraction of thin films allows it to detect strain relief and defect formation in thin epitaxial films, e.g. in SiGe high-speed devices. Total reflection X-ray fluorescence (TXRF) is able to detect surface impurities on wafers at levels of a millionth of a monolayer.

Recent advances at 3rd generation synchrotron radiation sources, such as the ALS, have made several new techniques feasible. These include impurity detection by resonant soft X-ray fluorescence (e.g. boron dopants in silicon) and a number of spectromicroscopy techniques. They allow it to detect not only the chemical variations across a surface or a device, but also to distinguish different bonding partners.

Photoluminescence of a Two Dimensional Electron Gas in the Quantum Hall Effect Regime

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In this talk we address recent progress in the study, by photoluminescence (PL) spectroscopy, of correlated two dimensional electron systems (2DES) confined in semiconductor heterostructures. In particular, we focus our attention on the investigation of these systems in either the integer quantum Hall effect (IQHE), the fractional quantum Hall effect (FQHE), or the Wigner Crystal regime. The IQHE and the FQHE are characterized by the fact that there exists no gapless excitations within the 2DES. Although the quantum Hall effects (QHE) have been discovered, and traditionally studied, by electric transport techniques, optical spectroscopy was sought as being a suitable instrument to unveil valuable information about the 2DES, and its many-body ground states, that could not be accessed by transport studies. In fact filling factor dependent "anomalies" - energy shifts of PL emission lines, decrease in the PL peaks intensity, appearance of new transitions, doublet or even multiplet structures for lower filling factors - were found in the PL spectra of a 2DES. The PL spectroscopy studies can be classified in two categories: experiments involving radioactive recombination to a hole localized in a plane containing acceptors atoms, and experiments in which the emission arises from the recombination of an electron (or quasi-particle) from the 2DES and an mobile (itinerant) hole. In the first case the experimental results are reasonably explained by current theory. The same is not the truth for the itinerant hole case, the main topic of this talk, where most experimental results still lack a good theoretical model. We review some experimental results and theories that have been put forward to account for the new spectral features, comment on new theoretical predictions such as "anyon excitons", and the possibility of detecting charge fractionalization by optical spectroscopy, and show that the behavior of a 2DES, as observed by optical spectroscopy, is strongly dependent on the distance between the 2DES and the holes. We present recent results that demonstrate how this important parameter can be controlled, and how the theory of magneto-roton mediated radioactive recombination, put forward to explain the doublet structure at $n = 1/3$, compares with our results. Several novel features observed in polarized photoluminescence from excitons in a spin-polarized GaAs quantum well near filling factor = 1 will be presented, together with a newly developed theory of PL recombination in the $n = 1$ regime, that incorporates the vision of filling factor as a strongly correlated electron system. We also comment on how controlling the electron-hole distance in PL experiments can help in finding solid experimental evidence for Wigner crystal formation at low filling factors.

POSTER SESSION I

AB INITIO CALCULATIONS OF CARBON-CARBON PAIRS IN SILICON

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Interstitial-substitutional carbon defect pairs (C_iC_s) in silicon display an interesting metastable behavior associated with two different structural configurations. In this work, we perform *ab initio* total energy calculations for this system on the neutral charge state. Our calculations are based on the pseudopotential, local-density-functional (LDA) and supercell approximations. Our results show that:

(i) The metastable configuration has C_{3h} symmetry and it is reminiscent of the isolated carbon-interstitial configuration, i.e. a split-interstitial C-Si pair (each atom three-fold coordinated). The substitutional carbon links to the silicon-interstitial.

(ii) The ground-state configuration also displays C_{3h} symmetry, but it consists of a single silicon-interstitial, two-fold coordinated in a bridge configuration between two substitutional carbon atoms. The two configurations agree with the ones suggested by experiments.

(iii) The ground-state configuration is lower in energy by 0.11 eV. The energy barrier for jumping from one configuration to the other is 0.13 eV. At higher temperatures, the stable configuration becomes a motionally averaged state with C_{3v} symmetry, corresponding to a rotation of the silicon-interstitial around a $\langle 111 \rangle$ axis. The calculated barrier for rotation is 0.07 eV.

(iv) Analysis of local-mode vibrations of the ground-state configuration indicates a stronger component in one of the carbon atoms. This behavior explains the experimentally observed isotope splittings.

MAGNETO-OPTICAL AND MAGNETIC RESONANCE INVESTIGATIONS OF INTRINSIC DEFECTS IN ELECTRON IRRADIATED N-TYPE $\text{Al}_x\text{Ga}_{1-x}\text{As}$

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Three intrinsic defects were observed in liquid phase epitaxy (LPE) grown n-type Te-doped $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ($x = 0.16$) after electron irradiation at low temperatures. With the magnetic circular dichroism of the absorption (MCDA) and the optical detection of electron paramagnetic resonance (ODEPR), two of these defects were identified as being an anti-structure-pair defect, $\text{As}_{\text{Ga}}\text{-Ga}_{\text{As}(\text{mm})}$, and the trigonally distorted gallium vacancy, V_{Ga}^2 ($g = 2.05$ and $\Delta B_{1/2} = 70$ mT for $B \parallel [100]$), also present in electron irradiated GaAs [1,2]. Although their ODEPR spectra showed no significant change when compared with those of the same defects in GaAs, their optical properties, reflected in the positions of the MCDA bands, were changed according to the increase of the bandgap. The third defect is not present in electron irradiated GaAs and was better observed in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ with additional illumination. While both the MCDA spectrum and the annealing dynamics are very similar as for the trigonally distorted V_{Ga} , the ODEPR spectrum is quite different. It is isotropic with $g = 2.048$ and $\Delta B_{1/2} = 50$ mT ($B \parallel [100]$). From the analysis of the ODEPR lineshape on the basis of the hyperfine interaction with the first As neighbors, for both the trigonal V_{Ga} and the new defect, we propose that the latter is also a gallium vacancy-like defect which is not trigonally distorted, probably because of the suppression of the static Jahn-Teller distortion in the presence of nearest Al neighbors.

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**AB INITIO ELECTRONIC STRUCTURE CALCULATIONS OF
ZINC-BLENDE InN**

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The Nitride compound semiconductors of group-III have been seen as good candidates for semiconductor devices which are active at wavelengths ranging from the blue to the UV. Recently, in order to obtain high power emission from UV to the yellow region in light emitting diodes, an InGa_N single-quantum-well structure has been used as active layer [1]. In their ground state structure, the nitride compounds appear as hexagonal wurtzite crystallized materials. However, the zinc-blende cubic phase of InN for example is often observed [2]. Despite the already existent experimental data on these materials, many of the fundamental properties of group-III nitrides are still not well established. In this work we perform rigorous *ab initio* total energy calculations of zinc-blende InN by using the self-consistent full potential Linear Augmented Plane Wave method (FPLAPW) within the large unit cell approach. The Indium *4d* electrons are treated as valence and also left frozen in the core. It is found that the explicit treatment of the In *4d* electrons as interacting valence states rather than inert core states systematically improves structural and electronic properties. The *d*-derived states appear as resonances in the InN valence-band close to its bottom. Including the *4d* as valence electrons also yields larger lattice constants in better agreement with experimental data. We also study the nonlinear hydrostatic pressure dependence of energy gaps, obtaining the linear and quadratic coefficients which can be compared with the experimental values.

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STUDY OF THE DIAMOND CRYSTAL BY SEMIEMPIRICAL METHODS

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Diamond is a technologically interesting material, and novel growth techniques (e.g. polycrystalline chemical vapor deposited (CVD) diamond^[1]) that produce material cost-compatible with other large-gap semiconductors have fostered the search for Carbon-based opto-electronic devices. Besides Diamond, there is an effort to combine organic conducting polymers, and new materials such as polysilanes^[2]. The theoretical study of complex or disordered semiconductor structures through *ab-initio* techniques, always difficult because of the large number of atoms that need to be included in a supercell, is hindered in the case of Carbon by the large number of plane waves that are needed in the basis set. An alternative is to apply semiempirical Quantum-Chemistry techniques, very successful for Carbon chemistry: the problem here is that the $s-p^3$ hybridization useful for Diamond-based structures enters with very little weight in the usual molecular parametrizations. We present a procedure for the study of structural properties of complex Carbon-based materials, consisting of an implementation of the self-consistent semiempirical MNDO/AM1 (Modified Neglect of Diatomic Overlap/Austin Model 1) for periodic systems in Bloch limit, within the supercell approach; and a new parametrization, which we call MNDO/Crystal, that is appropriate to the crystalline environment, but to be used also in the usual molecular code. This method was implemented in our group, but was parametrized only for Si^[3]. Our results for the diamond crystal are promising; for the lattice parameter we have an error of -1.4% compared to experimental results, while the numbers obtained with the original parametrizations of AM1 and PM3 (Parametric Method 3, the most successful variant of AM1 up to now) are -2.7% and -4.7% respectively. For the diamond bulk modulus, where the strenght of a method for predicting structural properties is best tested, we are able to obtain an error of 3.5%, as compared to 170% and 155% for AM1 and PM3, respectively. Of course, for the study of complex systems where charge density is more localised, it is very important that our parametrization attains sufficient accuracy when describing small molecules. We therefore tested our parameters in reproducing also the geometry (interatomic distances, angles) and vibrational modes of methane (CH₄), ethane (C₂H₆) and benzene (C₆H₆), among others. For all these molecules we have obtained results in good agreement with the experimental data.

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AB INITIO STUDY OF GROUP V ELEMENTS IN AMORPHOUS SILICON AND GERMANIUM

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When group V elements are introduced in tetrahedrally bonded amorphous semiconductors such as Silicon (a-Si:H) and Germanium (a-Ge:H) some interesting effects are observed. These effects are mainly related with transport properties. Nowadays, there is no doubt that impurities like N, P and As can act as effective n-type dopants in these semiconductors. However a reliable microscopic description concerning the behavior of these systems is still missing.

In the present work we report for the first time *ab-initio* calculations of the configurational and electronic structure of P-, As- and N-doped a-Si and a-Ge. The calculation procedure is based on two approaches. First, we have used the Monte Carlo (MC) method with the interatomic potential developed by Tersoff to generate the a-Si and a-Ge atomic configuration. Then, we have analyzed the electronic and structural configuration within the framework of the density-functional theory (DFT) with the local density approximation. The Kohn-Sham equations are solved using the Car-Parrinello scheme. Large unit cells and pseudopotentials were used and the single-particle electronic orbitals were expanded in plane waves with cutoff energy up to 45 Ry. All systems studied have been relaxed until the Hellmann-Feynman forces were lower than 0.01 eV/Å.

Based on the calculations described above, several interesting conclusions can be drawn. The main conclusions are: (i) The impurities are stable, for all the cases that we have studied, when 3-fold coordinated. (ii) In the case of these kind of impurities substituting 4-fold host atoms, the impurities are metastable. The conclusion (iii) is in conflict with the generally accept concept that 4-fold coordinated group V elements would not be stable in a-Si and a-Ge in the neutral charged state. But it permits a more convenient interpretation of n-doping experimental results in this kind of material.

PERSISTENT PHOTOCONDUCTIVITY IN P-TYPE Ge-DOPED AlGaAs

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The conductivity behavior as a function of the temperature, as well as the photoconductivity were investigated for liquid phase epitaxy (LPE) grown, p-type and homogeneous Ge-doped $\text{Al}_{0.4}\text{Ga}_{0.6}\text{As}$ layers. When cooling the sample in the dark, two distinct regimes of conduction were observed. The first, dominant at higher temperatures, shows an activation energy of 130 ± 10 meV which is very similar to the thermal ionization energy of the isolated Ge_{As} -acceptor, for $x = 0.4$ [1]. Below 100 K a hopping conduction regime in the Ge-impurity band becomes dominant. In this second regime, after illuminating the sample with light of energy below the band gap, a weak persistent photoconductivity effect (PPC) was measured. It was verified that the PPC is present up to 190 ± 10 K. In order to explain this PPC we suggest a model in which the metastability is caused by a lattice relaxation present in the ground state of the Ge-acceptor.

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ON THE STABILITY OF FULLERENE-LIKE $(\text{BN})_n$ CLUSTERSM.S.C. MAZZONI, H. CHACHAM

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Keywords: fullerenes, Hartree-Fock, electronic structure

We propose a family of fullerene-like clusters $B_{30+n}N_{30+n}$, with n from zero to six. $B_{36}N_{36}$ has only 4 and 6-membered rings and has the lowest total energy per atom. The reduction of n by one, in the family, eliminates a 4-membered ring and creates two 5-membered rings. This results in a "wrong" B-B bond and a "wrong" N-N bond, increasing the total energy per atom at the HF level. The resulting $B_{30}N_{30}$ in the family has a C_{60} -like topology with the smallest possible number of B-B and N-N bonds. This $B_{30}N_{30}$ cluster has also a total energy (at the HF level) lower than that of a $B_{30}N_{30}$ nanotube-shaped cluster. We also estimate that the energy necessary to create a pair of "wrong" B-B and N-N bonds by atom exchange in the $B_{30}N_{30}$ fullerene cluster is 4.3eV, at the HF level.

(CNPQ)

FIRST-PRINCIPLES CALCULATION OF SUBSTITUTIONAL OXYGEN AND OXYGEN-HYDROGEN COMPLEX IN GALLIUM ARSENIDE

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We have investigated the electronic structure, atomic geometry and formation energy of the isolated oxygen impurity (O_{As}) and the complex $O_{As}-H$ in GaAs with total energy pseudopotential calculations. This method are based on the density-functional theory (DFT) in the local density approximation (LDA), using a supercell approach with 32 atoms per cell. A soft norm-conserving pseudopotential are generated by the scheme of Troullier-Martins, transformed into the separable form of Kleinman-Bylander. The wave functions are expanded in a plane-wave basis set with a kinetic energy cutoff of 48Ry. Relaxation of two shells of host atoms around the impurities are included. We performed tests of convergence as a function of the plane-wave basis set and conclude that the cutoff energy used is adequated. The dispersion of the defect level was estimated in 0.1eV.

Our results for isolated O_{As} in neutral charge state, show an on-site defect with an a_1 midgap level occupied with one electron. No oxygen displacements from the arsenic position was observed, as shown our total energy curve as a function of the oxygen dislocation along $\langle 100 \rangle$ and $\langle 111 \rangle$ directions, for the neutral and negative charge states. This results was confirmed in calculations with 60Ry cutoff on 16 atoms supercell. There is an inward relaxation of the four neighboring Ga atoms, the O-Ga bond is 13% smaller than Ga-As bulk bond lenght. The atomic relaxation is accompanied by an energy gain of 1.1eV. The calculated formation energy shows that this defect can exist only in three charge states (+, 0 and -), the position of the transition levels under extreme Ga-rich condition were found in $(0/+)=1.02\text{eV}$ and $(-/0)=1.26\text{eV}$ above the top of the valence band.

For the neutral complex $O_{As}-H$, we calculated the total energy for several interstitial positions of hydrogen, we observed that the various configurations differ only slightly in energy. The most stable configuration emerging from our calculations has hydrogen in the center of $O_{As}-Ga$ bond. The bond-centered H is strongly bonded to O atom with bond length of 1.05Å, whereas the bond between H and Ga atoms is weak with bond length of 1.94Å. The hydrogen passivation of the impurity level is observed. We have also calculated the vibration frequency of the hydrogen atom for the wagging and stretching modes in a frozen phonon approach.

**ELECTRICALLY DETECTED SPIN-DEPENDENT RECOMBINATION IN
DELTA (Si) DOPED GaAs GROWN BY MBE AT LOW TEMPERATURE**

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Investigations of electrically detected magnetic resonance (EDMR) via spin-dependent recombination (SDR) in a delta doped (Si) GaAs sample grown by the molecular beam epitaxy at 300°C (LT-MBE) in a [311] direction have shown the signals due to an arsenic antisite-related defect. The sample consists of a delta doped region with a two dimensional Si concentration of about $N_{2D} = 3.4 \times 10^{12} \text{ cm}^{-2}$ within 0.2 μm of MBE GaAs grown at 300°C. The observed electrically detected electron paramagnetic resonance (EDEPR) spectrum shows the well-known quartet hyperfine split spectrum of an As antisite - related defect with a g - factor of 2.045 and a hyperfine splitting due to ^{75}As ($I = 3/2$) of 2600 MHz. The EDEPR parameter are very similar to those for the EL2 defect observed in bulk GaAs. Optically detected magnetic resonance (ODMR) investigations in similar grown MBE GaAs have shown high concentrations of As antisite-related defects [1]. Whether these defects belong to EL2 or another As antisite-related defect is not the matter of the present discussion. In this contribution we concentrate our discussion on the mechanism which can be responsible for the observation of the EDMR spectrum in terms of spin-dependent recombination processes, i.e. donor - acceptor recombination and the role of spin polarization effects. The observation of an As antisite-related defect in this n-type GaAs under illumination is only explainable in terms of spatially separated carriers. The present discussions are important for the investigation of other devices based on III-V semiconductors.

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Electronic Structure of Erbium-Oxygen Impurity Pairs in Silicon

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The electronic structure calculations of erbium-oxygen impurity pairs in silicon have been carried out by using the self-consistent-field multiple scattering theory within the framework of the molecular cluster model. The *quasirelativistic* theory in which the radial functions inside each atomic sphere satisfy an average Dirac equation that includes the Darwin and mass-velocity corrections, but not spin-orbit term, has been used.

As the geometry of the cluster is determined by the location of the defect, the substitutional Er-substitutional oxygen and interstitial Er-substitutional oxygen impurity pairs have been simulated by clusters containing 71 and 72 atoms, respectively, having 36 hydrogen terminators, both in trigonal symmetry.

The Er 4*f* and 6*s* states have been treated as valence states. The calculated results do not support the assumptions that the 4*f* electrons could be treated as a frozen core. The results also show that some kind of hybridization among 4*f*, 6*s*, 5*d*, and 6*p* orbitals takes place in the interaction between Er and silicon host atoms.

STUDY OF CONFORMATIONAL DEFECTS ON ORGANIC SEMICONDUCTORS: POLYACETYLENE AND POLYCARBONITRILE

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Organic semiconductor have attracted a great amount of attention over the last two decades ever since the discovery that, the simplest conjugated polymer (polyacetylene) can be controllably doped so that its electrical conductivity can be varied over twelve orders of magnitude [1-3] from insulator to metal. Undoped polyacetylene is an insulator because it undergoes a pairwise distortion introducing alternating single and double bonds thus creating a band gap in the electronic π system. As the pairing distortion has defects in it, one can find a finite density of localized states at the Fermi level [4], and the metallic regime, with suppression of bond alternation, is only obtained at a very high dopant concentration [5]. It is currently accepted that, due to the electron-phonon coupling present in these conjugated systems, local distortions of the chemical bonds occurs on the chains in order to store the transfer charge from the dopants species to the polymer. These defects species are commonly referred to as solitons, polarons and bipolarons and play an important role in the electronic properties of the semiconductor, as seen for instance in optical-absorption measurements and in transport properties. It was shown [6-8] that a disordered distribution of such defects may be able to produce a metallic band structure with extended states at the Fermi level, then fulfilling the requirements to find an insulator to metal transition.

An exemple of such a system is the so called polycarbonitrile. This class of polymer was synthesized more than 20 years ago [10] by heating polyacrylonitrile to about 200 °C and conductivity measurements indicated semiconducting behavior [11]. Even though trans-polycarbonitrile shows many similarities with trans-polyacetylene, it is not clear that polycarbonitrile can be considered a synthetic metal.

In the present work we report a theoretical study on the effect of the presence of conformational defects like soliton, polaron, bipolaron on the electronic properties of polyacetylene-polycarbonitrile copolymers. Negative Factor Counting and inverse interaction techniques have been used to evaluate densities of states and wave functions, respectively. Our results show a finite density of state at the Fermi energy for high defect concentrations. This fact, together with the extension of the highest occupied molecular orbital (HOMO) state, indicate the possibility to have the copolymer in the metallic regime.

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NEUTRON TRANSMUTATION DOPING OF SILICON AND OTHERS SEMICONDUCTOR MATERIALS

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The doping of semiconductor materials is of crucial importance in determining their final properties such as the resistivity. The Neutron Transmutation doping (NTD) of semiconductor materials is a way of doping in which the quantity of dopant material can be precisely controlled and homogeneously distributed throughout all the material. Samples such as a small thin films up to large single crystal can be irradiated in a nuclear reactor.

The NTD method is based on a nuclear reaction where some nuclei of the semiconductor material capture thermal neutrons and form unstable radioactive nuclei which beta decay to nuclei of a different element. Since the resultant element has at least the atomic number $Z = \pm 1$, where Z is the atomic number of the starting material, it belongs to one of the neighbouring columns (in the periodic table) to that of the start element, hence it is a N or P type dopant. In silicon, for example, nuclei of the ^{30}Si isotope ($\sim 3.1\%$ of natural silicon) capture thermal neutrons producing ^{31}Si nuclei which decay to the stable isotope ^{31}P which is a N type dopant. Irradiation of Germanium with neutrons produces Ga (P type), As (N type) and Se (N type) dopants simultaneously, while in the case of Ga(As) the NTD produces both Ge and Se dopants with ratio of Se and Ge concentration of $N_{\text{Se}}/N_{\text{Ge}} = 1.46$. Since the Se and Ge atoms are expected to act as donors, NTD produces mainly N-type Ga(As).

This work presents a short review of the NTD technique and the experiments of silicon irradiation performed at the IEA-R1 research reactor in São Paulo, where an irradiation rig with simple design has been constructed and installed. The rig permits the irradiation of silicon crystals with diameter up to 4 inches. By adopting a procedure in which two ingots 25 cm long each are irradiated simultaneously and their positions interchanged at a point when precisely half the total necessary neutron dose has been received, it has been possible to achieve the desired axial uniformity of the neutron dose. This method avoids the use of neutron absorbing shields around the crystals which necessarily compromise the overall irradiation capacity of the reactor. Test irradiations were performed with 100 float zone silicon crystals and the results of radial and axial uniformities in the final resistivity values as well as the doping accuracy obtained show an excellent doping quality achieved.

**DEFECTS CHARACTERIZATION OF
IRRADIATED SOLAR CELLS
USING TRIGONOMETRIC WEIGHT FUNCTIONS**

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This paper describes a method to treat capacitance transients in solar cells using trigonometric weight functions. The method is based on the Deep Level Transiente Spectroscopy (DLTS) technique using a single or a double lock-in as the integrator module. It is shown that any combination of sinusoidal and cossinusoidal functions with the same period of the repetition pulse can be used as a weight function for defect detection purposes. Lock-in amplifiers conceived as alternate voltage meters can be used in this measurement.

Three weight functions are discussed in detail: $F(t) = \sin(\omega t)$, $F(t) = \cos(\omega t)$ and $F(t) = \sin(\omega t) - \cos(\omega t)$. The sensitivity and resolution of the method are determined and compared with the main variations of the DLTS technique. Experimental data are discussed for defect levels in p-n junction silicon solar cells produced by irradiation of 1 MeV electrons with fluences varying from 1×10^{12} to 1×10^{15} el/cm². This work shows that the DLTS peak temperatures can vary in a range of 20K depending of the chosen weight function. Depending on the temperature range of the experimental set-up, the choice of the weight function is fundamental to the detection of defects.

**COMPLEX-DEFECTS RELATED WITH ELECTRICAL
ISOLATION BY ION-IRRADIATION IN n-GaAs:
A THEORETICAL STUDY**

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We report calculations of the electronic structure of complex-defects, neutral and charged, in GaAs. Particularly, we are interested in defects that are created during light ion implantation, which plays a fundamental role in the development of the III-V compound semiconductor technologies. A theoretical study is presented using a full *ab initio* method adopting the supercell approach in Car-Parrinello scheme. A supercell with 128 atoms, Bachelet-Hamann-Schlüter-type pseudo-potentials is used in the calculations. Our results show that complex $\text{Ga}_{\text{As}}\text{-As}_{\text{Ga}}$ (Ga-antisite + As-antisite) and $\text{V}_{\text{Ga}}\text{-Ga}_{\text{As}}\text{-As}_i$ (Ga-vacancy + Ga-antisite + As-interstitial) defects introduce a deep-level acceptor with a localized state below the middle of the semiconductor band gap. The defect-reactions in the different annealing stages are discussed to explain the observed changes in the resistivity.

MULTIPHONON ASSISTED TRANSITIONS OF METASTABLE HOLES GENERATED BY STRONG NEAR BAND GAP LIGHT IN GaAs

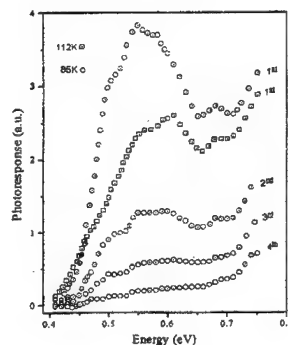
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Key words: Multiphonons, Metastability, Holes, GaAs:O,

We have studied photo conductivity properties in GaAs nominally doped with oxygen under strong exposure to illumination in the temperature range 40K to 300K. During the process of inducing photo quenching effects, we have also observed a metastable population of holes which are created after samples exposure to near band gap light. Its lifetime is not so sensitive to temperature as it is for the photoquenching processes. The time decay dependence on the temperature for such a population of holes, shows an activation energy of 33.8meV for the low temperature regime (below 80K) and a deactivation of 42.9meV for temperatures up to 200K. The difference between these values gives 76.7meV which establishes the presence of a negative potential barrier to electron capture into these centres. Such a barrier has been reported in slow domain formation studies in GaAs[1]. We observe clearly three sources of photoresponse above the valence band at 0.54eV, 0.60eV and 0.67eV respectively. The photo excitation of these holes shows a structure which may be explained by a multiphonon assisted process. We have been able to fit the electronic transition assisted by 0.03eV phonons for each one of the levels with poissonic distributions. The response also includes contributions of electrons being excited from a level 0.48eV below the conduction band. This however, is easily observable only after exposure to strong illumination. We put forward a simple model relating these features to the presence of $X_{Ga}-Y_i$ impurity complexes where X may be an As or a vacancy and Y may be an As or O. We also make an effort to explain the metastable photo excitation for the population of holes based on a level to level transition throughout a shallow acceptor level 0.03eV above the valence band.

Photoresponse after exposure to 1.4eV light. Scans are take with a narrow slit. Numbers mean the chronological order for subsequent scans. One can notice four peaks roughly at 0.50eV, 0.54eV, 0.60eV and 0.67eV.



ELECTRONIC STRUCTURE OF POINT DEFECTS IN SiC

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Recently, the progress in CVD and MBE techniques for the controlled growth of cubic Silicon Carbide(3C-SiC) started a rapid development of SiC-based devices, which are suitable to work under extreme conditions such as high temperatures and pressures. It is well known that point defects are responsible for a good(or not) electronic performance of such devices, and they can appear at high concentration when stoichiometric deviations occurs during the SiC growth. In this work, we have calculated the electronic structure of the point defects on this material. To do that, we have used the Molecular Cluster Model within the framework of the *ab initio* LCAO-MO Unrestricted Hartree-Fock method in the *Gaussian92* code. The following point defects were studied: vacancies, anti-sites, Si and C interstitials at both tetrahedral and hexagonal sites. Our results show good agreement with both experimental findings and other theoretical calculations, whenever these comparison are possible. From the total energy evaluation, including relaxation and local distortion effects, our results show that the vacancies and the anti-sites are the most energetically stable point defects found in 3C-SiC grown by the deposition techniques.

PACS indexes: 71.55.-i, 71.55.Hi, 31.20.Di

Keywords: Semiconductors, Electronic Structure, Point Defects

ON THE ORIGIN OF PHOTOLUMINESCENCE FROM InAs/InP SYSTEMS: THE
COMPETITION BETWEEN 2D STRUCTURES AND 3D ISLANDS

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In this work we investigate the electronic properties of InAs/InP systems, grown by Chemical Beam Epitaxy, using low temperature photoluminescence(PL) and Atomic Force Microscopy(AFM). In this lattice mismatched system three dimensional coherent islands are formed - in the Stranski-Krastanow growth mode - which coexist with the wetting layer, an essentially two-dimensional system. We show that the morphology of the InP surface just before InAs deposition strongly affects the characteristics of these systems. Smooth surfaces - typically obtained from two-dimensional growth mode - and periodical multi-terrace structures -originated from three-dimensional growth - were used as buffer layers to evaluate this effect. Samples grown simultaneously on (100) InP substrates nominally-oriented and 2° off towards different directions (A, B and C-surfaces), present remarkably different behaviors. These differences are related to the process of redistribution of InAs film, at the InAs/InP interface. We analyze the PL emission originated from the InAs wetting layer, which consists of few monolayers, considered as a very thin quantum well. PL spectra with multiple-peaks are observed for structures deposited on (100) and A-surfaces. These results indicate that the corresponding wetting layers present different thickness along the structure. On the other hand, all samples grown on substrates containing B-steps (B and C-surfaces), present spectra dominated by a single peak which is characteristic of a more uniform wetting layer. The PL line widths are relatively small (~15meV) and are attributed to short range interface roughness, i.e., smaller than the exciton diameter. We analyze these results considering how the diffusion of surface atoms on different types of surfaces and different morphologies affect the redistribution of the InAs layer. We base our discussion on the AFM observation that presence of natural steps and intentional corrugations play important role in this process.

**CHARACTERIZATION OF p-TYPE Si-DOPED SEMICONDUCTING
STRUCTURES GROWN BY MOLECULAR BEAM EPITAXY ON (3,1,1)A
GaAs SUBSTRATES**

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P-type doping of semiconductors is very important for micro- and optoelectronics industry to make NPN junction transistors or PN junctions for optical emission or detection. GaAs based materials (GaAs, InGaAs and AlGaAs) are generally grown on top of (100) GaAs substrates as they are easy to clean quimically and to be cleaved along one of the natural cubic axis. The production of p-doped samples is generally realized by simultaneous evaporation of Be atoms that incorporate into the Ga site, leading to a deficiency of one electron per impurity atom. However, Be-doped samples have several drawbacks: Be atoms are much smaller than Ga and As atoms and can diffuse over long distances into the host material; as a consequence sharp p-type doping profiles, especially planar doping, are very difficult to obtain. In addition, beryllium is unefficiently evacuated by conventional pumping, yielding a possible background contamination of posterior samples.

In this work, we are reporting on the use of (311)A GaAs substrates and Si evaporation to produce p-doped samples. Under special growth conditions (580-600 °C growth temperature, low As/Ga flux ratio), the Si atoms enter the As site, leading to a p-type doping. Si-doped p-type samples behave much better, as silicon has a diffusion length almost 100 times smaller than beryllium and can be pumped out of the system very quickly. Several sets of samples have been grown by molecular beam epitaxy (MBE) in order to optimize the growth conditions of this kind of system (substrate temperature, As/Ga flux ratio, dopant concentration as a function of cell temperature). Characterization of the epitaxial layers has been done by Hall effect and photoluminescence. Very sharp excitonic peaks of the GaAs layers grown on top of a (311)A substrate have been obtained, demonstrating the high quality of the growth process. Several types of heterostructures (quantum wells, planar doping) have been grown simultaneously on top of (100) and (311)A substrates and will be compared.

High index-plane substrates offer new possibilities of growth techniques due to the presence of natural steps. These substrates are also good candidates for producing low dimensional structures (quantum dots and wires) that are now becoming of huge interest for optoelectronics.

GROWTH AND CHARACTERIZATION OF $\text{In}_x\text{Ga}_{1-x}\text{P}$ ON GaAs BY CHEMICAL BEAM EPITAXY

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$\text{In}_x\text{Ga}_{1-x}\text{P}$ is lattice-matched with GaAs when $x \cong 0.5$. We have grown and analyzed undoped and doped $\text{In}_x\text{Ga}_{1-x}\text{P}$ with x varying around 0.5. In this work we present the characterization results. We have obtained Hall carrier concentrations as high as $2 \times 10^{19} \text{cm}^{-3}$ for Si-doped (n-type) samples but, for those doped with Be, the highest concentration without surface deterioration was about $5 \times 10^{17} \text{cm}^{-3}$. Beyond this value, we have found for InGaP layers, the same behavior as heavily Be-doped InP layers.

The gap variation with composition shows a transition that seems to have its origin in the ordering effect.

In order to test the confiability of our growth calibration, we have fabricated some devices and the results will be presented here.

Utilization of a four layer resist process to examine the effects of asymmetric gate recess on InGaAs/GaAs PHEMTs

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The DC and microwave characteristics of two sets of InGaAs/GaAs PHEMTs (power high electron mobility transistor) are compared. The first set is composed of devices fabricated using a trilayer electron beam resist process for T-gate recess and metallisation. The second set is composed of devices fabricated using a new four layer resist process which enables the asymmetric placement of a T-gate in a wide recess trench. Characteristics are compared for devices whose gate length is 0.2 μm and whose extent of cap recess on the drain side of the gate (L_{ud}) varies from 0 to 0.55 μm . It was found that the devices showed an overall improvement in the characteristics necessary for high power applications as L_{ud} was increased. For example, the off-state drain-source breakdown voltage increased from 5.5 to 12.5 V, the voltage gain increased from 16 to 57, and f_{max} increased from 133 to 158 GHz as L_{ud} was increased from 0 to 0.55 μm .

Adsorption and dimer exchange process of As₂ molecule over GaAs:Te, GaAs:Se and GaAs:S surfaces

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We have performed first-principles calculations for the adsorption of As₂ molecule over GaAs:Te, GaAs:Se and GaAs:S (001) surfaces. Considering (2x2) and (4x2) surface reconstructions, we investigate the dimer exchange process between the adsorbed As₂ dimer and sublayer chalcogen atom.

Beginning with a monolayer of Te atoms over GaAs (001), Ga terminated surface, we have observed that the adsorption and a subsequent exchange process between As₂ (adsorbed) molecule and the Te sublayer is an exothermic process, indicating the surfactant nature of the Te atoms on As layer [1]. The second As₂ adsorption, that is an exothermic process, but the subsequent exchange process is not. On that way, Only half a monolayer of Te atoms segregate to growth surface. This partial surfactant action of Te is confirmed by Rodrigues et al. [2], but is in contrast with the dimer exchange of the In atoms, where we verified that Te atoms are completely surfactant to then [3]. Starting with half a monolayer of Te atoms over GaAs (001), Ga terminated surface, we obtain an adsorption energy -0.91 eV/dimer smaller than an adsorption over a monolayer of Te atoms, but the subsequent exchange process is not energetically favorable. That result point out that Te atoms (at coverage of half a monolayer) do not segregate to the growth surface by dimer exchange process. For the Se covered surface with a monolayer and half a monolayer, the As₂ adsorption process is an exothermic process. In the half a monolayer coverage the adsorption energy for the As₂ molecule is 0.70 eV/dimer smaller than with a monolayer coverage of Se, but in both structures the dimer exchange process is not energetically favourable. This results confirm the stability of GaAs:Se covered surface not favoring the As ↔ Se exchange process. The As₂ molecule adsorption on a S covered on GaAs (001), Ga terminated surface, is an exothermic process. Again like on the Se coverage, the subsequent dimer exchange process is not energetically favourable, and also confirm the stability of GaAs:S surface against an As ↔ S exchange process. Comparing the adsorption energy of As₂ molecule on the Te, Se and S covered GaAs (001) surfaces, we observe that this energy is proportional to the difference of eletronegativity between the surface chalcogen atom and the As atom. Also this energy is proportional to the deformation of the As₂ adsorbed molecule (dimer bond-length). The following table present the adsorption energy, dimer bond-length (As-As), and As-{Te,Se or S} exchange energy, for the As₂ adsorption on GaAs: {chalcogen} (001) surface:

structure:	E ^{AD} [eV/dimer]	d _{As-As} ^o [Å]	E ^{exchange} [eV/dimer]
GaAs:Te	-1.92	2.37	-0.11
GaAs:Se	-2.48	2.51	+0.84
GaAs:S	-3.14	3.93	+1.17

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**IS THERE A COMMON LIMITING STEP IN DIAMOND GROWTH
ACTIVATION ENERGY?**

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In this paper we present the measurement of the activation energy for diamond chemical vapor deposition from carbon tetrachloride mixtures in a hot-filament assisted reactor. Mixtures of 1 vol% CCl₄ in H₂ have been used in most experiments. Growth rates have been measured in the temperature range from 220 to 820 °C to obtain the activation energy. Raman spectroscopy and Scanning Electron Microscopy show that crystalline diamond was obtained only for substrate temperatures over 420 °C. We also present an extensive comparison with most activation energy determinations in the literature and propose that there is a common trend in most observations, independently of the gas mixture used, with or without the addition of oxygen or halogens.

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**DETERMINATION OF GAS PHASE REACTIVE SPECIES IN CHLORINE
ASSISTED HOT-FILAMENT CHEMICAL VAPOR DEPOSITION OF
DIAMOND BY MASS SPECTROMETRY.**

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In this study we work with carbon tetrachloride as a carbon source for diamond growth in a hot-filament chemical vapor deposition system. This compound has interesting characteristics in relation to methane: lower bond strength in C - Cl than in C - H; possibility of diamond growth at lower temperatures due to a lower activation energy; higher efficiency in surface reactions due to the easy of hydrogen abstraction by chlorine radical.

The experiments were performed with 1 vol% CCl₄ in H₂. The mixture was made passing part of the hydrogen flux through a bubbler with CCl₄. There were two gas inlets, one remote, placed on the top of the reactor, and one local, placed close to the substrate position. The substrate was substituted by a quartz microprobe for local gas collection for mass spectrometry analysis. The quartz microprobe had a 200 μ m collection orifice. The distance from the filament and the tip of the quartz microprobe was 5 mm.. The distance between the local gas inlet and the quartz microprobe tip was varied from 2 to 4 mm.. Three gas inlet combinations have been tested: remote and local feeding of the mixture, and remote hydrogen feeding with local feeding of the CCl₄. Three different filament temperatures have been tested: 1375, 1625 and 2125 °C.

The results of our experiments show that at 2125 °C the carbon tetrachloride is almost completely dissociated and converted into hydrocarbons, mainly methane and acetylene, and HCl, independently of the gas inlet configuration. Similar results are observed at 1625 °C, but with the local gas inlet at 2 mm from the microprobe tip the dissociation of CCl₄ is not complete. Intermediate C2-chlorine radicals and probably some *m/e* species, derived from CCl₄, appear with local gas feeding at a filament temperature of 1375 °C. Also, some CH₃Cl (*m/e* =50) was found for gas inlet at 2 mm from the microprobe tip. All results suggest that the contribution of chlorinated hydrocarbon radicals for diamond growth is very unlikely. The fast conversion of CCl₄ into hydrocarbons suggests that the growth mechanism is via methyl radical. Growth experiments have been analyzed by Scanning Electron Microscopy (SEM) and Raman Spectroscopy.

SELF-ASSEMBLED InAs ISLANDS MORPHOLOGY AND ITS EFFECT ON THE InP BUFFER LAYER

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Significant research effort has been devoted to study the growth of self-assembled islands in strained heterostructures, due to its potential as a maskless technique for fabricating quantum dots. The formation of islands is based on the transition from 2-D to 3-D growth driven by a partial elastic relaxation within the islands.

We investigate the formation of thin films of InAs on InP by Chemical Beam Epitaxy. The InP buffer layer was grown on kinetic limited conditions that results in an intentionally corrugated surface. The surface presents elongated channels along a preferential direction. The cross-section of the channels shows a sawtooth-like profile.

This work focus on the evolution of the InAs film morphology and its effect on the InP layer underneath. We have followed the effect of annealing on As atmosphere subsequent to the InAs deposition using both microscopic (Atomic Force Microscopy) and optical (Photoluminescence, Excitation Photoluminescence and Raman spectroscopies) techniques. The Atomic Force Microscopy results showed the redistribution of InAs on the InP surface. We observed the formation of 3D islands. Their distribution is strongly affected by the presence of channels in the InP buffer layer. As we increase the annealing time, coarsening process takes place, resulting in fewer but larger islands. The optical properties of the structures show a clear dependence on the InAs morphology. This dependence is also observed in the InP emission, including the excitonic and the shallow impurity regions. For instance, we observed that the annealing procedure results in the appearance of an extra InP emission line, usually attributed to P vacancies.

MOUNDS IN GaAs HOMOEPITAXY: FORMATION AND EVOLUTION

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Although the basic mechanisms of epitaxial growth on flat singular crystal surfaces have been studied for a long time, new scenarios for the morphology of homoepitaxial films have been reported recently. In particular, it has been observed that the morphology of homoepitaxial films of several materials takes the form of well-defined three-dimensional mounds. In this work, we report the dependence of surface morphology of GaAs homoepitaxial films on growth parameters: mound formation and evolution are observed to occur under certain conditions. The morphologies were analyzed with Atomic Force Microscopy (AFM). The GaAs films were grown by Chemical Beam Epitaxy using triethylgallium (TEG) and thermally-cracked arsine as group III and V precursors, respectively. (100) GaAs substrates with nominal orientation and 2° off towards $\langle 110 \rangle$ direction were used.

The morphology of the GaAs substrates after oxide desorption presents a high density of pits with depth as large as 10nm and a smooth surface between them. The grown films, on the other hand, present a morphology typical of two-dimensional growth, with rms roughness $\sim 0.3\text{nm}$. In such morphologies, typical features from annealed samples, like wide terraces and step bunching, are not observed on the films grown on nominal substrates. Instead, we observe terraces with circular (isotropic) shape forming in some cases well-defined mounds. For 300nm-thick samples a larger density of mounds is observed when the sample is grown with larger TEG flows. In this case, a drastic reduction in the mound size occurs. For thicker films, however, the morphologies observed for samples grown with different TEG flows are similar, showing wider terraces. This indicates that a coarsening process takes place during growth, increasing the overall area of the mounds; the terraces in this case are still isotropic in shape. The same morphologies are observed for vicinal substrates though the terraces in the mounds are not resolved in this case. The dependence on TEG flow, thickness and growth temperature suggests that these initial structures are related to the surface observed after oxide desorption and form in the process of surface healing: planarization of the surface is favored by conditions which enhance surface diffusion.

IMPROVEMENT OF THE STRUCTURAL PROPERTIES OF NEAR STOICHIOMETRIC PECVD SiO_2

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Abstract

In this work we present the improvement on the compositional and structural properties of silicon dioxide films deposited by direct plasma enhanced chemical vapor deposition (DPECVD) from gaseous mixtures of N_2O and SiH_4 . The studied films were deposited at substrate temperatures of 320 °C, SiH_4 flow of 3 sccm, rf power density of 250 mW/cm² and always keeping the residence time on the minimum value permitted by the deposition system. In order to determine the structural characteristics, we use the FTIR and Ellipsometry techniques.

It is known that the frequency of the stretching vibration of the Si-O bond is related with the bond angle and with the stoichiometry of the material. Also, it has been shown that the thermal relaxation of the films deposited by remote PECVD is very different from thermally grown films [1].

We have obtained SiO_2 films with a stretching vibration frequency for the Si-O bond very close to the thermally grown SiO_2 one [2]. We observed also that increasing the $\text{N}_2\text{O}/\text{SiH}_4$ flow ratio, the frequency of stretching vibration of the Si-O bond increases, becoming even closer to the Si-O stretching vibration position in thermally grown SiO_2 . Furthermore, we can see that the absorption peak of the stretching vibration of the Si-O bond out phase (region established between 1100 and 1200 cm⁻¹) presents a better definition. These results indicate that an appropriate increase in the $\text{N}_2\text{O}/\text{SiH}_4$ flow ratio will produce more stoichiometric films and a bond angle similar to the thermally grown SiO_2 . Studies on the thermal relaxation of the films are on the way to verify this hypothesis. Also the results of our late depositions show this tendency, even though for the highest tested value of the flow ratio a decrease in film stoichiometry was obtained, which was attributed to the significant increase of undesirable gas phase reactions due to the enhanced deposition pressure. For this reason, in our next experiments we will increase the flow ratio by decreasing silane flow in order to keep the deposition pressure low, avoiding the gas phase reactions.

The measured values for the refractive index and for the deposition rate of the films also demonstrate that increasing the flow ratio, the refractive index decreases, while the deposition rate remains constant. These results are consistent with a better stoichiometry of the films.

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KINETIC LIMIT OF SEGREGATION DURING THE MOLECULAR BEAM EPITAXY OF GaAs/AlAs HETEROSTRUCTURES

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The segregation of cations during the molecular beam epitaxy (MBE) of III-V semiconductor heterostructures causes nonabrupt interfaces and thus limits their structural quality. So far a thermodynamical equilibrium model has been frequently used to account for the segregation [1]. This model treats the process of exchange of cations between the bulk and the surface. According to the prediction of the thermodynamical model the segregation increases when the temperature decreases, but this contradicts the experimental observations [2,3]. A recently proposed kinetic model [4] enables to take into consideration the growth rate; when the growth rate is greater than the exchange contributions the segregation becomes proportional to the growth temperature.

The model developed in [4] takes into account the exchange of cations which takes place between the last *already completely formed* surface monolayer and the bulk phase considered as the previous monolayer. We however suppose that, because of the low enough growth temperature used in MBE, the exchange reaction between the already completely grown surface monolayer and the bulk may not be significant. In this case the exchange of cations occurs *during the growth of the surface monolayer* between the monolayer which is in process of growth (the surface phase) and the last grown one (the bulk phase).

In our model we used these considerations in order to correct the kinetic model presented in [4]. As a surface phase we examine the two-dimensional nuclei known to be an initial phase of the monolayer growth. Our corrections assume critical conditions (the growth temperature and the growth rate) for a kinetic limitation of the MBE growth strongly dependent on the form of the two-dimensional nuclei; with the same growth rate the kinetic limitation occurs at a higher temperature than the predicted in [4].

A good agreement was found between the compositional profiles obtained by Raman scattering of the optical phonons in the GaAs/AlAs superlattices [3] and those calculated by our model.

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THE CARBON INCORPORATION IN PECVD α -Si_{1-x}C_x:H IN THE LOW POWER DENSITY REGIME

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Abstract

In previous works it was shown that the "silane starving plasma" regime, a particular case of the low power density regime, has fundamental importance for the growth of α -Si_{1-x}C_x:H thin films with very special characteristics, as chemical order similar to c-SiC and wide gap material with diamond like properties¹.

In this work we study the carbon, silicon and hydrogen incorporation in α -Si_{1-x}C_x:H thin films obtained by radio frequency (rf) plasma enhanced chemical vapor deposition (PECVD) in the rf low power density regime in and out of the "silane starving" conditions. The Si, C and H content were obtained by Rutherford Backscattering (RBS) and Forward Recoil Spectrometry (FRS), and the chemical bonding of those elements were studied by Fourier Transform Infrared spectroscopy (FTIR).

The results show that, conversely to what has been suggested by other authors for the low power density regime², for films grown in the starving regime, the carbon content in the solid phase (x) can be larger than 0.5, a value of 0.7 was obtained for a methane concentration of 95% in the gaseous phase. Also the main carbon bonds are not C-H₃ but sp³ C-H₂ and Si-C.

Other important result is that despite the very high hydrogen concentration, increasing from 35 a.t. %, for very low carbon content samples, up to 50 a.t. % for all the samples with x > 0.3, the [H]/[C] ratio (calculated by RBS) decreases from more than 4 for Si rich samples to less than 2 for carbon rich films. This result makes the hypothesis of carbon incorporation as methyl groups unprovable for high carbon content samples, which is reinforced by the fact that the [C-H₃]/[C] ratio (calculated by FTIR) is less than 0.2 for samples grown in the "silane starving plasma" regime.

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Differential gain analysis of InGaAs/InGaAsP/InP multiquantum well lasers with 1.55 μm emission wavelength

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Long wavelength semiconductor lasers emitting at 1.55 μm are very important for applications in high speed and long haul optical communications. In order to operate with good performance characteristics, such devices usually present high differential gain and high external quantum efficiencies. These parameters are strongly dependent on the material properties of the active layer and on the epitaxial structure of the active region, as well as on leakage current of the device. The latter has been shown recently to affect the material gain/current-density characteristics (1). In this work, we have investigated laser devices comprising a separate confinement heterostructure (SCH) with multiquantum well (MQW) layers grown in the InGaAs/InGaAsP/InP material system. The epitaxial structure was grown by MOCVD, and consisted of 6 InGaAs QW layers of about 70 \AA thickness and InGaAsP barrier layers corresponding to 1.3 μm emission wavelength with 130 \AA thickness. The waveguiding layers of the SCH were 645 \AA thick and had the same composition as the barrier layers. Both ternary and quaternary layers were grown lattice matched to InP. The devices were processed as broad area lasers with various cavity lengths in the range 350-700 μm . The measured threshold current densities were around and below 2KA/cm². The differential gain was determined from the cavity length dependency of the threshold current density, using a simple and approximate expression as a function of the carrier density. The effects of the leakage current in the device structure were also taken into account in the analysis of the laser static characteristics. The results obtained are consistent with previous reported data for the differential gain employing other measurement techniques.

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SECONDARY ION MASS SPECTROMETRY ANALYSIS OF Be INCORPORATION IN InGaP.

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Be incorporation in $\text{In}_x\text{Ga}_{1-x}\text{P}$ ($x \cong 0.49$) samples grown by Chemical Beam Epitaxy, CBE, at a temperature of 535°C , was analyzed using Secondary Ion Mass Spectrometry, SIMS, and Hall measurements. The results show that despite the carrier (hole) concentration saturates at around $3 \times 10^{18} \text{ cm}^{-3}$, in our case, the Be concentration reaches values higher than this, indicating that part of the Be is not electrically active. It was also observed a Be accumulation in a region close to the surface, for samples grown under the highest Be fluxes used in the present work. This is indicative that, at this growth temperature, the solubility of Be in InGaP has reached its limit.

GROWTH OF InGaAs QUANTUM DOTS BY MOLECULAR BEAM EPITAXY

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For more than 20 years, molecular beam epitaxy (MBE) has been one of the best tools for producing 2D semiconductor systems (quantum wells, superlattices). However, lower dimension features (quantum wires and dots) were generally achieved by post-growth *ex-situ* nanolithography, as a consequence of the severe restrictions for MBE growth. A few years ago, several groups pointed out a new and easy way for producing *in-situ* quantum wires and dots that lead to an intense study of such systems. This kind of structures are very important for optoelectronic industry that needs small, homogeneous and ordered nanostructures to be able to fabricate high-efficiency microlasers.

In this work we are reporting on the growth of InGaAs quantum dots on GaAs substrates by the self organization method. A strained layer of InGaAs material is grown on top of a GaAs substrate, and mesoscopic structures (the quantum dots) appear when the critical thickness of the layer is slightly exceeded, which mainly depends on the In content and growth temperature. Several sets of samples were grown, varying the growth temperature, In content and strained layer thickness in order to study the influence of the growth parameters on the morphology and electronic properties of these nanostructures. Higher In concentrations yielded sharper 2D-3D RHEED transition (streaky to spotty pattern) that was much easier to detect than for lower In concentrations. However, for such high In contents, the growth temperature had to be lower down to 480 °C to avoid the use of a too high As flux and In re-evaporation.

Each sample consisted of a 0.5 μm GaAs buffer, a 60 Å of low In-content quantum well, a 1000 Å thick GaAs layer, a thin high In-content InGaAs layer, and a 300 Å thick GaAs cap layer. The 60 Å quantum well acted as a reference for photoluminescence measurements. The thickness of the second InGaAs layer was varied from one monolayer below the critical thickness up to one monolayer above the critical thickness. PL measurements showed a broad peak at higher energy (higher than expected for a quantum well of the same width), related to the formation of the quantum dots. Special samples, without any cap layer and reference quantum well were also grown to carry out STM and AFM measurements in air using a new sample preparation developed in our lab. These measurements showed that the dots had an average size and height of 400 Å and 100 Å respectively and were randomly distributed on the surface. Growth on (100) vicinal (2°, 4°, 6° off) or on (311)A substrates are in progress to investigate the possible ordering of these dots along the steps running on the substrate surface.

STRUCTURAL CHARACTERIZATION OF PHOTOLUMINESCENCE POROUS SILICON WITH FTIR SPECTROSCOPY

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This paper presents an analytical model proposed to determine morphological parameter of porous silicon layer using results obtained with the Fourier Transform Infrared characterization techniques.

Porous silicon layer was obtained from Boron - doped (100) silicon of 20 Ω cm resistivity with HF 48% (w/o) aqueous solution at current density ranging from 5 mA/cm² to 15 mA/cm² [1]. Using the proposed model, it was found that porous silicon layers have porous size of 6.6 nm, specific surface of 600 m²/cm³ and the residual crystal size about 3.7 nm. Dots in the porous silicon (3.7 nm) have apparently a quantum confined behavior [2]. This fact is confirmed with the photoluminescence behavior of the sample that presents photoluminescence peak at 725 nm.

After an anodically oxidation with KNO₃ [3], the porous silicon layer presents a blue shift of 75 nm on the photoluminescence peak. Variation observed on the emission, is verified using the proposed model with parameter extracted from Fourier Transform Infrared characterization. The shift of photoluminescence is interpreted as the result of more quantum confinement.

These experimental results encourage the model proposed as a tool to characterize the porous silicon morphology.

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**VERTICALLY STACKED SELF-ASSEMBLED
InGaAs QUANTUM DOT LAYERS GROWN
ON (311)A/B AND (001) ORIENTATIONS**

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In this work, we present the substrate orientation effects on optical properties of vertically stacked $\text{In}_{0.5}\text{Ga}_{0.5}\text{As}$ quantum dot (QD) layers grown by molecular beam epitaxy on (311)A/B and (001) GaAs substrates. Samples were grown with different GaAs spacer layer thicknesses. The spacer thickness variation shows influence on photoluminescence (PL) spectra for all surfaces. The differences in integral luminescence, peak shape, position, and amplitude have also been observed for all planes. PL peak shifts to lower energy and spectral linewidth decreases compared with the single set of islands. This behavior indicates coupling between the electronic states of these QD layers. Quantum dot's anisotropy is also indicated by PL polarization measurements.

INTRINSIC AND DOPED MICROCRYSTALLINE SILICON FILMS FOR APPLICATION IN DOUBLE BARRIER STRUCTURES

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ABSTRACT

In this paper we present experimental results on the preparation and characterization of intrinsic and n-type doped $\mu\text{c-Si:H}$ films, with the aim of obtaining a high mobility intrinsic material and a good electron injecting contact for application in devices as superlattices and double barrier devices, TFT's, etc. The samples were prepared by the direct PECVD method from gaseous mixtures of ($\text{SiH}_4 + \text{H}_2$) for intrinsic material and from ($\text{SiH}_4 + \text{H}_2 + \text{PH}_3$) for n-type doped samples. It is known that a correct balance between etching and deposition is the key for obtaining microcrystalline silicon by the PECVD technique¹, in this way the SiH_4 flow rate, the hydrogen dilution ratio, and the rf power were changed to optimize this balance ratio. All the samples were grown at a substrate temperature of 300 °C and the films were characterized by optical absorption measurements, Fourier Transform infrared spectroscopy, X-Ray diffraction, and electrical measurements. The primary results show that by selecting a suitable rf power, a low SiH_4 flow rate, and a high hydrogen dilution ratio, intrinsic $\mu\text{c-Si:H}$ films have been obtained, with grain size as large as 130 Å, determined from X-ray diffraction measurements. Larger grain size is expected for samples deposited under the optimized deposition conditions whose x-ray characterization is on the way.

In order to obtain n-type $\mu\text{c-Si:H}$ films the phosphine concentration in the deposition gaseous mixture was varied, maintaining the other parameters identical than for the intrinsic material. A very high doping efficiency was observed, even for PH_3 concentration as low as 0.28%, a conductivity of $1.52 (\Omega\cdot\text{cm})^{-1}$ was obtained. It was observed that high PH_3 concentrations prejudice the material grain size and even the electrical conductivity, indicating a decrease in mobility. The IR absorption of $\mu\text{c-Si:H}$ films, which corresponds to the amorphous phase at the grain boundary, is an indication of the crystalline fraction of the material. For samples deposited under optimized conditions, very low absorption intensity of Si-H_n ($n = 1,2$) was observed, suggesting a high crystalline fraction for these samples.

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EFFECT OF THERMAL ANNEALING ON $a\text{-Si}_{1-x}\text{C}_x\text{:H}$ DEPOSITED UNDER SILANE STARVING PLASMA REGIME

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ABSTRACT

In this work we present the resolution the effect of thermal annealing in $a\text{-Si}_{1-x}\text{C}_x\text{:H}$ deposited by the PECVD technique in the low power regime in and out of the silane starving plasma condition. Details on the deposition conditions are described elsewhere¹. The thermal annealing were done for 2 hours in intervals of 50 °C from 350 °C up to 1100 °C. The characterization was done by Fourier transform Infra Red (FTIR) spectroscopy, analyzing the evolution of the absorption bands corresponding to the vibrations of main hydrogen bonds as well as the fundamental SiC bond.

Both the physical and the structural response to the heat treatments of starving deposited samples showed important differences with non- starving deposited samples. The former ones presented better adherence to the substrate, were more resistant to thermal stress and showed less densification. Non-starving produced samples on the contrary suffered a pronounced decrease in thickness after the first annealing and pop out completely after a few heat treatments. For this reason in order to analyze the response of non-starving samples to higher temperatures much thinner films had to be deposited. Respect to the structural behavior, we observed that hydrogen from both, CH_n and SiH_n bands effuses at lower temperatures from non-starving produced films suggesting weaker bonds. As an example the SiH_n vibration in non starving samples began to decrease at 330 °C and disappeared completely at 550 °C while for starving samples the decrease began only at 450 °C and the disappearance occurred at 700 °C. Also non-starving samples it showed an increase in the CH_2 and CH_3 bands for the first annealing which was attributed to the increase in films density. In starving samples a continuous decrease of the bands was observed. All samples presented a shift in the SiH_n band from 2090 cm^{-1} to 2040 cm^{-1} which reinforces the theory that the 2090 cm^{-1} band is due to SiH vibration in a cluster environment.

Finally the evolution of the band at 780 cm^{-1} confirmed that it is due to SiC stretching vibrations instead than to $\text{Si-(CH}_n\text{)}$ as has been reported². The evolution of these band was very different for both type of samples, specially at the lower temperature steps. As deposited starving samples already present a large band at this frequency while non-starving samples do not, in this way the effect of the annealing steps in the former was just a slow increase and narrowing of the band. Non-starving samples instead show important variations which embrace a huge increase of the SiC band together with a diminishing of the vibration band at $\text{Si-(CH}_n\text{)}$ 1000 cm^{-1} and the SiH band at 640 cm^{-1} .

¹ I. Pereyra & M.N.P. Carreño, Journal of Non-Cryst. Solids **201**,110 (1996).

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GROWTH OF InAs QUANTUM DOTS ON GaAs MEDIATED BY Te

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The control of size, distribution, and shape of islands on Stranski-Krastranov heteroepitaxial growth is a major goal for fabricating self-assembled quantum dots. Surfactants offer an opportunity to master the epitaxial growth of such structures. Surfactants proved to change growth modes completely. They also proved to reduce dislocations in heteroepitaxial growth. Dislocations are claimed to play the major role on self-assembled quantum dot non-radiative recombinations and thus they reduce the luminescence yield. Here we study the role of Te as a surfactant in InAs/GaAs heteroepitaxial growth by means of atomic force microscopy (AFM) and reflection high energy electron diffraction (RHEED).

A series of samples of InAs deposited on GaAs with different coverages of Te and InAs were grown by MBE. The samples were grown with a buffer layer of GaAs to improve the crystalinity of the substrate surface and to avoid dislocations to propagate from the substrate inside the growing islands of InAs. Some samples of GaAs covered with Te were also produced to make Rutherford Backscattering measurements (RBS) to find the dependence of Te coverage on the GaAs surface with temperature.

AFM measurements were done on the samples in air after growth, using a Nanoscope III from Digital Instruments Inc. . With the aid of a computer program we could make statistics on height, radius, and density of the islands on the samples.

Te showed strong influence on InAs islands density, height, and radius. We were able to increase island density and diminish the size in the range of 1.6 to 2.3 ML by letting 0.3 ML of Te on the GaAs surface. We also observed a transition between two configurational states of the InAs islands in the observed range.

DOPING EFFICIENCY IN HIGHLY ORDERED PECVD $a\text{-Si}_{1-x}\text{C}_x\text{:H}$

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ABSTRACT

Recently we have pointed out the importance of the "silane starving plasma" condition on the optical, chemical and structural properties of $a\text{-Si}_{1-x}\text{C}_x\text{:H}$ obtained by standard radio frequency Plasma Enhanced Chemical Vapor Deposition (PECVD) technique from Silane (SiH_4) and Methane (CH_4) gaseous mixtures. We have shown that in this condition is possible to obtain, an almost stoichiometric material ($x \sim 0.5$), a chemical and structural order similar to crystalline SiC and, for carbon rich material ($x > 0.5$), very high optical gap ($E_o \sim 4$ eV) and other "diamond like" properties, as high electrical resistivity and resistance to chemical etching ^{1,2}.

In this work we study the effect of the "starving plasma" condition on the electrical transport properties and on the N-type doping efficiency for both, near stoichiometric and carbon rich $a\text{-Si}_{1-x}\text{C}_x\text{:H}$ material. In this way we measure properties as dark conductivity, photoconductivity, activation energy and carrier mobility ($\eta\mu\tau$ product) of the samples. The doping of the samples was obtained by Ion Implantation of Phosphorous and Nitrogen and at this moment we are preparing samples doped *in-situ* by the addition of phosphine (PH_3) and nitrogen (N_2) or Ammonia (NH_3) to the gaseous mixture. Preliminary results have shown that the intrinsic samples do not present important photoconductivity. On the other hand we observed a high doping efficiency for both dopant elements, phosphorous and nitrogen, obtaining an increase of 5 orders of magnitude in the conductivity for phosphorous doped samples and of 4 orders of magnitude for nitrogen doped ones.

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² V. Mastelaro, A.M. Flank, M.C.A. Fantini, D.R.S. Bittencourt, M.N.P. Carreño and I. Pereyra, Journal of Applied Physics, vol 79 (3) pg.1324, 1996.

VERY LOW HYDROGEN CONTENT $a\text{-Si}_{1-x}\text{C}_x\text{:H}$ DEPOSITED UNDER
SILANE STARVING PLASMA REGIME

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ABSTRACT

In previous works we have shown that PECVD films deposited under silane starving plasma conditions have very interesting and particulate properties, among them, close to stoichiometry samples exhibit a chemical order similar to c-SiC. It is this last property which motivated the search for appropriated deposition conditions for obtaining micro-crystalline material ($\mu\text{c-SiC:H}$) by the PECVD technique. It is known that a correct balance between etching and deposition is the key for obtaining $\mu\text{c-Si:H}$ by this technique¹, the balance is achieved for high RF power and high hydrogen dilution. This concepts have been applied to a-SiC but the result was a material consisting of Si μc embedded in an a-SiC:H tissue.

In this work we use our knowledge on obtaining ordered a-SiC almost stoichiometric in order to use it as a starting material to explore higher rf power and increasing H_2 dilution². In this way we started a sample series using the same deposition parameters than for stoichiometric a-SiC:H but adding H_2 to the gaseous mixture. The other series was done keeping the hydrogen dilution at the optimum value and increasing the rf power density. The samples were characterized by Fourier transform infra-red spectroscopy and profile measurements, X-ray diffraction measurements are on the way to determine the existence of micro-crystals. The results show that increasing rf powers and increasing hydrogen dilution promote the growth of a material with enhanced density of Si-C bonds and with a much lower hydrogen concentration. It is also observed that the etching process attacks preferentially the C-H_n sites, in this way in order to obtain stoichiometric material higher methane concentrations should be utilized either for increasing rf power density or hydrogen dilution. The analysis of the width and shape of the SiC band for the sample deposited at the highest rf power density suggests the onset of crystallization. This sample also showed negligible density of CH_n bonds.

¹ C.C. Tsai, G.B. Anderson and R. Thompson, Mat. Res. Soc. Symp. Proc. Vol.192, p475.

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NATURAL OXIDATION OF POROUS SILICON

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This work reports the evolution of the chemical species at the porous silicon (PS) surface monitored by Fourier Transform IR (FTIR) spectroscopy. The room temperature visible photoluminescence (PL) from PS samples were characterized, too.

Porous silicon layers were formed on lightly p-doped (100) oriented silicon substrates by anodisation at constant current density ($J=20\text{mA}/\text{cm}^2$) in electrolytes composed of 50% aqueous hydrofluoric acid and 50% ethanol or only of aqueous hydrofluoric acid (48%wt). The sample named "PS1" was formed with HF/ethanol for 5min; PS2 was formed with HF for 10min and PS3 was formed with HF/ethanol for 20 min.

In this study the effects of natural oxidation on these samples are reported. They were in a desiccator for the whole period of the analysis (ten months), but they were in air as measured.

It is noted that the Si-O and Si-H_x-O bonds increased in the aging process, but the hydrogen surface coverage was preserved. A progressive decrease in the band of Si-H_x groups and an increase in the absorption of the oxidized Si-H_x groups were observed (Fig.01). The integrated area of the Si-H_x peaks remains constant (Fig.02).

The characterization of the Si-H_x stretching modes gives an idea of surface area in these samples as function of the time of anodisation.

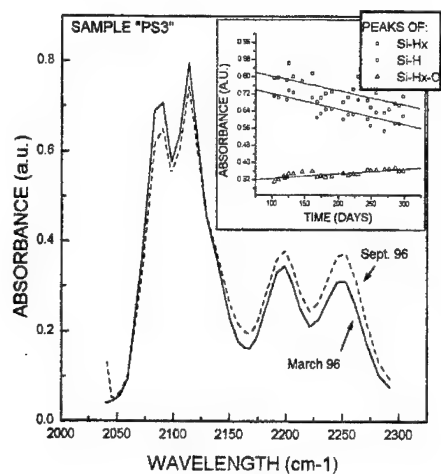


Figure 01

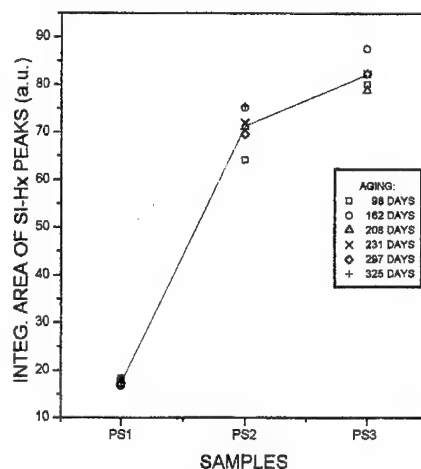


Figure 02

FILLING GRAPHITIC NANOTUBES

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The hollow interior of fullerenes and related materials have attracted a great deal of interest as it could be used to generate new encapsulated compounds. In particular, nanotubes¹ represent an remarkable high aspect-ratio object ($\approx \mu\text{m}$ in length, and ≈ 10 nm in diameter), that could be used as template for the fabrication of nanowires. An simple method to fill nanotubes, is based on the capillarity properties of these nanostructures^{2,3}. Here, we report a study of capillary driven filling of carbon nanotubes by molten salts. Nanotubes were first opened by oxidation, subsequently annealed to 2000 °C, and finally immersed in molten silver nitrate. Although, a majority of the tubes tips are open, capillarity filling displays a low efficiency ($\approx 2\text{-}3\%$), and only for inner cavity diameters ≥ 4 nm (while cavity size distribution peaks at ≈ 2 nm). This observed size dependence of capillarity forces, is attributed to a rehybridization of the sp^2 -like carbon atom bonds with decreasing diameter. A simple model is proposed, which allows the interpretation of the results⁴ and moreover chose potential candidates for nanotube capillarity filling⁵.

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BAND RENORMALIZATION AND INTERVALLEY SCATTERING IN NEAR BAND GAP FEMTOSECOND OPTICAL PROBING OF ALGAAS NEAR THE Γ -X CROSSOVER

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Ultrafast interaction of carriers with their environment is a central problem for the understanding of many fundamental properties of semiconductors. Experiments investigating these effects provide valuable information for subjects ranging from the development of high speed electronic devices to fundamental questions in many-body and plasma physics¹.

Here we present femtosecond absorption saturation measurements in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ alloys with x near the Γ -X crossover (~ 0.43). Relatively less is known about the ultrafast carrier kinetics in indirect-band-gap materials than direct gap semiconductors. Recent work on Ge² has shown the variety of phenomena revealed by ultrafast spectroscopy in indirect gap semiconductors: band-gap renormalization, carrier-carrier scattering, carrier cooling and intervalley scattering.

The time resolved photoinduced transmission experiments are performed in the usual pump and probe geometry. Pulses of a colliding pulse mode-locked dye laser with a wavelength of 620 nm are amplified to a energy of 1 μJ in a six-pass dye amplifier pumped by a 5.6 KHz cooper-vapor laser. Part of the amplified pulses (2.02 eV, 100 fs) is focused in a 10 mm fiber to generate a "white-light" continuum (1.91 eV to 2.14 eV, 30 fs) which covers the spectral vicinity of the alloy gap, while the rest of the energy goes to the pump pulse (2.02 eV).

For a sample with $x = 0.43$ ($E_G^\Gamma = E_G^X \cong 1.98$) if we probe the photoinduced changes at 2.06 eV after excitation at 2.02 eV we observe an initial bleaching that decays to a constant value in 500 fs. Most interesting results appear when we use a probe pulse with a energy of 1.94 eV. In this case, like recent work of Mack et. al. in Ge we see an instantaneous increase of absorption due to instantaneous band gap renormalization induced by the excited Γ carriers. This is followed by a bleaching (mainly due to state filling) and a ultrafast bleaching decay due to the scattering of the carriers to the side valleys. It is interesting to see that the carriers injected at 2.02 eV fill the states at 1.94 before being scattered to the side valleys.

Another interesting feature of the signal is that after about 500 fs there is a small recovery of the bleaching to a constant value. We have modelled these data considering that carriers renormalize differently according to the energy valley which they occupy. As the carriers scatter to the side valleys they contribute to renormalization of the energy of the carriers in central valley only through correlation and no more also through screening-exchange interaction³. This leads to a partial recovery of the bleaching due a recovery of the Γ gap energy. Similar results are obtained studying a indirect sample ($x=0.48$, $E_G^\Gamma = 2.02$, $E_G^X = 1.99$ eV) when we probe at 2 eV following excitation at 2.02 eV. These experiments provide original information about the femtosecond dynamics of the direct gap in highly excited AlGaAs in this special context: the presence of lower energy accessible side valleys.

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OPTICAL INVESTIGATION OF INTERDIFFUSION IN NARROW GaAs/AlAs QUANTUM WELLS

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GaAs/AlGaAs heterostructures and quantum wells are widely used in optoelectronic devices. The quality of these devices strongly depends on the abruptness of the composition change at the interfaces. Diffusion of Ga into the AlAs barrier and Al into the GaAs well during growth smears out the step-like change of composition and alters the optical characteristics of these structures.¹ A controlled intermixing of Ga and Al can be used as a technique for integration of different devices.² Therefore the exact knowledge of interdiffusion parameters is of great importance for device development.

We have employed photoluminescence spectroscopy to experimentally study the effect of atomic interdiffusion on the optical properties of narrow GaAs/AlAs single quantum wells. The well widths of the quantum wells grown by LP-MOVPE vary between 6 and 20 monolayers (17 Å and 56 Å, respectively). Different diffusion profiles at the interfaces were induced by thermal annealing each sample at a fixed temperature for different periods of time.

The photoluminescence spectra show a blue shift of the transition energy with increasing diffusion length as well as a nonlinear decay of the luminescence peak intensity. In addition, beyond a critical diffusion length L_c , the luminescence can no longer be observed. L_c is strongly correlated to the width of the quantum well.

The observed features are explained by a transition from direct-gap to indirect-gap behavior of the structure with increasing diffusion length and are in close agreement with tight-binding model calculations by Koiller et al.³

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MICRO-RAMAN ANALYSIS OF MINORITY PHASE ON CUBIC/HEXAGONAL GaN STRUCTURES

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The binary nitrides are nowadays the most promising materials for light emitting device in the blue/ultra-violet spectral region. Among them, GaN seems to be the best candidate. When grown on GaAs substrate, the GaN epilayer has a unique feature of being possible to crystallize either into wurtzite (hexagonal) or into zincblende (cubic) structures, depending on its growth conditions. The cubic phase is obtained using N-rich condition in the initial stage of deposition, whereas the hexagonal phase by a slight excess of Ga condition. In this work we have, by means of micro-Raman analysis, identified a minority hexagonal phase on cubic GaN samples, grown by a modified MBE system with rf activated plasma nitrogen source. Scanning electron microscope (SEM) photographs of these samples revealed the presence of some clusters of size of about two microns. Using micro-Raman experiments (~ 1 microns of spot diameters) we have identified that these clusters were micro-crystal with a defined crystalline phase. For cubic GaN one has just the LO and TO optical phonon, the latter being forbidden in the back scattering configuration. For hexagonal structure the predominant allowed modes are one $A_1(\text{TO})$ and E_2 optical phonons. Thus, identifying the Raman response we can identify the crystalline structure of the region from which it is taken. When the spot was positioned on the zone free of clusters the Raman signal shows the expected two peaks associated to the LO and TO modes of the GaN cubic phase. However, when the spot was positioned at the cluster a strong E_2 phonon frequency of the hexagonal phase was detected. A small peak at the E_2 -position was also present in the spectra taken from the cluster-free-zone, indicating that there are a small hexagonal material region also in this zone.

OPTICAL PROPERTIES OF TETRAGONAL HgI_2 AND ITS RELATIONSHIP WITH CRYSTALLINE QUALITY

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Mercury iodide is a tetragonal red semiconductor with a relatively large band gap of 2.13 eV at 20 °C. The recent growth (also on space shuttles) of single crystals of HgI_2 have been motivated by the important applications in photocells, room temperature x-ray and γ -ray radiation detectors and spectrometers, due to the large band gap (low noise), high resistivity, large average atomic mass and lifetimes of both electrons and holes. In particular, special attention have been given to the interesting properties of excitons in this material, such as, the very narrow luminescence emissions (less than meV), the high value of the free-exciton binding energy (≈ 35 meV) and the possibility of obtaining Bose-Einstein condensation in such materials. However, there still remains many material and processing issues that are of concern for further development and application.

In this work we present the main low temperature photoluminescence (PL) features of excitons in HgI_2 related with its crystal and electronic structures. We also try to establish a connection between optical properties and stoichiometry and impurity content of the material. The crystals used in our investigation have been grown from the vapor phase through the method of physical vapor transport in a properly evacuated ampoule. This method has been used to produce bigger crystals with superior quality than others. Before the growth, the starting materials were submitted to purification procedures, which consist of repeated sublimation cycles in a special designed ampoule. These procedures were also monitored by photoluminescence.

As expected, the results show that the success of growing good quality single crystals depends strongly on the purification cycles of the starting materials. We found that three purification cycles are sufficient to obtain high purity samples, as demonstrated by the very intense, well resolved and intrinsic excitonic emissions in the PL spectra. PL features related with impurities and iodine (mercury) deficiency are almost absent in high quality samples. These sole luminescence lines of tetragonal crystals depend on the orientation of the electric field vector of the incident radiation with respect to the c-axis of these crystals, and are assigned to free-exciton and their phonon replicas. Temperature dependent measurements show strong and symmetrical emissions even at high temperatures (200 K), in contrast to other semiconductors, which present a very asymmetrical high energy Boltzman tail. Detailed discussion of the PL measurements will be presented. In this work we will also show the results of growing ternary alloys of $\text{Hg}_x\text{Pb}_{1-x}\text{I}_2$ and the defect formation due to the lost of stoichiometry during the thermal processes.

INELASTIC LIGHT SCATTERING DUE TO COUPLED PLASMON-PHONON MODES IN δ -DOPED SEMICONDUCTORS

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In recent years, there have been many studies on the intersubband collective excitations of a two-dimensional (2D) electron gas and their coupling to the longitudinal optical phonons in semiconductor quantum wells and superlattices. The δ -doped polar semiconductors, such as Si δ -doped GaAs, have advantages to study the plasmon-phonon coupling because: i) the high electron density in the system and, typically, several subbands are populated; ii) the intersubband plasmon frequencies are close to the optical phonon frequency and their coupling can be strong; iii) the host material of the 2D electron gas is homogeneous and, as a consequence, the phonon modes have a three dimensional character; and iv) due to the spatial symmetry of the system, intra-intersubband mode coupling becomes unimportant.

In this work, the intensity of inelastic light scattering is obtained within the random-phase approximation for the multisubband system of Si δ -doped GaAs. The collective excitations and their coupling to the optical phonons are studied and the effects of the level broadening induced by impurity scattering on the spectra are analysed. We have varied the electron density in the range of 0.5×10^{12} to 10^{13} cm^{-2} . The calculations are based on the self-consistent solution of the subband electronic structure and wave functions.

We show that the high electron density leads to a large depolarization shift of the intersubband plasmon frequencies of the two adjacent subbands. Furthermore, both intra- and intersubband plasmon modes are strongly coupled to the optical phonon modes. With a small level broadening, we can find all the scattering peaks of different coupled intra- and intersubband plasmon-phonon modes. We also see that each mode is Landau damped only in its own single-particle continuum region. On the other hand, due to high impurity concentration in the real system, level broadening strongly modifies the inelastic light scattering spectrum and only a few scattering peaks can be observed. But such a damping does not affect the phonon-like modes pronouncedly. The scattering peaks from the phonon-like modes still can be clearly distinguished even with large broadening.

**PHOTOLUMINESCENCE OF Ge ISLANDS GROWN BY ULTRA HIGH
VACUUM -CHEMICAL VAPOUR DEPOSITION ON Si(100)**

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The morphology and size distribution of low dimensional structures have a crucial importance for indirect bandgap materials, since both the higher density of exciton localizing sites and the stronger confinement due to the reduced dimension lead to higher luminescence yields. Ge heteroepitaxy on Si follows a Stranski-Krastanov type of growth. The changeover between two dimensional (2D) coherent growth to 3D islanding has been recently related to clear modifications in the photoluminescence (PL) spectra [1,2]. Specifically, an emission band red-shifted with respect to the PL signal of the 2D strained layer, which can be observed when the critical thickness for pseudomorphic growth is overcome, has been identified as a 3D island-related structure.

In this work different Ge on Si samples have been investigated with respect to their morphology and optical properties. Ge was deposited on Si(100) by Ultra High Vacuum-Chemical Vapour Deposition from GeH_4 , without cap layer, at substrate temperature between 325-450 °C, using deposition rates as low as a few Å/min. Microscopic characterization showed that films with thickness ≤ 10 nm exhibited isotropic undulations due to round-shaped islands uniformly covering the substrate and having a narrow diameter distribution peaked between 45 and 50 nm. These samples were excited by the 514 nm line of an Ar^+ laser and the PL signals were detected with a 0.25 m monochromator followed by a cooled Ge detector with the standard lock-in technique. A PL band centered at 850 meV was observed at 12 K, which closely resembled the island-related feature observed for Ge dots embedded in Si. The PL spectra as a function of temperature and laser power density will be presented and discussed in terms of the morphological characteristics of the different samples.

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EXCITATION PHOTOLUMINESCENCE AND RAMAN SCATTERING IN SI-PLANAR DOPED GaAs

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Conventional photoluminescence is not useful for the investigation of planar doped semiconductors because the photogenerated electron-hole pairs are spatially separated from each other in a time ($\sim 10^{-13}$ s) much shorter than the recombination time ($\sim 10^{-10}$ s). Consequently one can observe only the emission occurring in the regions far from the doped plane, where the band bending is neglectable. We have demonstrated the utility of excitation photoluminescence to observe the electronic levels in those structures. Resonance in the absorption in the doped region enhance the emission of the exciton line in the flat bands regions. We also investigated the resonant raman scattering from the electronic excitations in the 2D electron gas in the doped region. Samples with multiple planes of doping were investigated and the experiments were performed at the temperature of 10 K.

**PHOTOREFLECTANCE AND TIME RESOLVED PHOTOREFLECTANCE IN
DELTA DOPED SUPERLATTICES (δ -Si:GaAs)**

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In this paper we report a detailed study of PR in δ -Si:GaAs superlattices. It is shown that PR spectra yield three contributions: (1) from intrinsic GaAs, (2) FKO due to the surface electric field, whose value is explained by a simple capacitor model and (3) FKO attributed to the buffer/superlattice interface. We observed the photovoltaic effect due to the probe beam in the PR arrangement and achieved surface voltage reductions up to 30%. We also present a new time resolved PR technique, which allow us to discriminate these contributions in the time domain and give us the PR characteristic decay times. The main advantage of this technique is that exhibits the whole PR spectra in the energy domain, but delayed with respect to the modulation. Time resolved PR showed that the first contribution has the longest response time (≈ 1 ms), while recombination processes responsible for FKO from surface electric field are faster (≈ 40 μ s) and can be explained by the Shen model¹. We interpret the faster characteristic decay times as the carriers recombination time between the first delta-doping plane and the surface states. Additional support for that is given by Raman scattering from coupled plasmon-LO phonons also performed in our samples, which show that only the first delta doped layer is depleted. Contribution (3) is very weak and it was not possible to attribute it a reliable response time.

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Optical measurements of InAs self-assembled quantum dots made by surfactant mediated growth with Te.

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Photoluminescence and absorption measurements were made on InAs self-assembled quantum dots which were grown on (100) and (311)A GaAs substrates, with and without a Te submonolayer coverage. The samples without Te showed typical luminescence response in the range of 1.1 to 1.35 eV. A faint signal was observed on the Te covered (100) sample and only at 10 K. On the other hand, a significant response was measured on the Te covered (311)A sample. A computer simulation was done in order to resolve the eigenenergies of both the hole and the electron on the dot. Absorption measurements showed, in comparison to quantum well structures, what seems to be a high quantum efficiency in the luminescence process.

PHOTOLUMINESCENCE AND MOBILITY OF SINGLE AND PERIODICALLY Si δ -DOPED InP GROWN BY LP-MOVPE

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Since it was proposed in 1980 [1], the δ -doping technique which would ideally confine the dopants to a single layer contributed much both to the understanding of fundamental properties of 2D systems [2,3] and to the development of high performance devices [3].

Most of the work in this field has been done on the GaAs and AlGaAs systems [3]. Net charge distributions with a full width at half maximum (FWHM) around 40Å for Si δ -doped GaAs layers have been measured by C-V profiling. Such a charge distribution implies in a dopant localization over 10Å or less, essentially reaching the ideal goal. Similar results were obtained for AlGaAs. However, few reports of other Si δ -doped III-V semiconductors are yet available [4]. Periodically δ -doped layers, several δ -doped layers separated by the same distance, have raised much interest due to their great potential for unique device applications. Such structures are attractive in the quest for high conductivity.

For applications and integration of devices operating at 1.55 μ m, the knowledge of the characteristics of single and periodically δ -doped InP based materials is of paramount importance. Thus, a systematic investigation of the transport and optical properties of single and periodically Si δ -doped InP structures with 5 and 10 periods varying from 100 Å to 300 Å, grown by LP-MOVPE, has been pursued.

A FWHM for the net charge concentration profile of 32Å was obtained for a sample with a peak net charge concentration of $1.8 \times 10^{19} \text{ cm}^{-3}$. Numerical simulations showed that for these samples the impurities are localized over not more than two monolayers. No dopant diffusion or segregation was observed. A reduction in mobility with decreasing period was obtained due to the increasing overlap of the electronic wavefunction with the various Si planes. A broad band emission was detected for the periodic structures at energies higher than the InP band gap. The cutoff energy for this band decreases with the period, d , and this behavior can be described by a $d^{-2/3}$ decay. This dependence can be understood as the dependence of the Fermi level position on the barrier width for the different samples.

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MODULATION-DOPED FIELD-EFFECT PHOTODETECTORS

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Since the advent of epitaxial growth techniques such as MBE and MOCVD, heterostructure and superlattice based devices have been attracting a great deal of attention. In this work it is discussed the photodetection properties of one of these structures, the MODFET (Modulation Doped Field Effect Transistor).

The main motivation for the present study is the possibility of exploring the multifunction capabilities of these phototransistors, beyond those offered by conventional photodiodes. Specifically, photodetection and amplification can be combined in a single monolithic structure, potentially simplifying the optical receiver configuration.

The devices investigated were pseudomorphic structures, fabricated under cooperation with Martin Marietta Electronics Laboratories (Syracuse/USA). On top of a semi-insulating GaAs substrate the following layer sequence was grown by MBE [1]: 1 μm of GaAs buffer, 100 Å of $\text{In}_{0.17}\text{Ga}_{0.83}\text{As}$ channel, 45 Å of undoped $\text{Al}_{0.17}\text{Ga}_{0.83}\text{As}$ spacer, 400 Å of doped $\text{Al}_{0.17}\text{Ga}_{0.83}\text{As}$ (Silicon planar doped $2 \times 10^{12} \text{ cm}^{-2}$) and 350 Å of heavily doped GaAs cap layer.

Our experimental results show that the MODFET photoresponse is characterized by a logarithmic dependence on light intensity and extremely high optical gain at low optical power levels, where a external quantum efficiency in excess of 10^5 A/W was recorded (i.e., 1 nanowatt of incident optical power produces more than 0.1 mA of output photocurrent). The results above were explained by solving Poisson and continuity equations and taking into account the quantum mechanical nature of the 2-DEG channel. According to this model [2], the action of the heterojunction built-in electric field on the photogenerated carriers produces two dominant effects:

- 1) a photoconductive mechanism, caused by photoelectrons which reach the 2-DEG channel and are collected by the drain terminal.
- 2) a photovoltaic mechanism, due to the built up of photogenerated holes, which are swept towards the high resistivity semi-insulating substrate. In steady state, this positive charge accumulation is counterbalanced by the injection of thermal equilibrium electrons from the source into the 2-DEG channel, producing the optical gain mentioned above.

The existence of these two mechanisms is verified by measuring the frequency spectrum of the photoresponse. The device displays two distinct time-constants, the first in the Mhz range, associated with the photovoltaic effect, and the second, related to the photoconductive effect, beyond 1.0 Ghz.

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PHOTOLUMINESCENCE STUDIES IN STRAINED Si SINGLE-DELTA DOPED InGaAs/GaAs HETEROSTRUCTURES

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Precise control of the spatial distribution of dopants has become important in fabricating high-performance semiconductor devices. Therefore, there is an interest in understanding the effects of the proximity of various kinds of semiconductors surfaces and interfaces to doped regions from both fundamental and applied perspectives. In this work, using photoluminescence (PL) measurements, we investigated the optical properties of several strained $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$ samples containing a single-doping layer of Si atoms located at different distances (d_{buffer}) from the GaAs(buffer layer)/InGaAs heterointerface. The samples analysed in this work were grown by a Gen II Mod. MBE system on EPI-ready (100) GaAs substrates with the following structure: a 0.5 μm GaAs buffer layer, a variable thickness layer (d_{buffer}) of $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$, a single Si delta-doped layer with an intended dopant density of $1 \times 10^{12} \text{ cm}^{-2}$ and a 2000 Å-thick layer of $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$ followed by a 50 Å GaAs cap layer. A series of samples with the single Si delta-doped layer located at a nominal depth $d_{\text{buffer}} = 100, 200, 300, 1000$ and 2000 Å from the GaAs(buffer layer)/InGaAs heterointerface was studied.

Besides various GaAs-related emission structures which arise from the GaAs buffer and cap layers, the luminescence from the InGaAs layers consists of a single peak in the energy region around the $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$ band gap, which shift to lower energy as the InGaAs layer thickness increases. This shift in the position with increasing thickness is also accompanied by a decrease in the full width at half maximum (FWHM) and a gradually increase of the intensity of the InGaAs peak. These results are in marked contrast with the dramatic decrease in intensities observed in the PL spectra in InGaAs/GaAs single heterostructures. The observed InGaAs-related emissions observed in the PL spectra of the three thinner InGaAs samples can be assigned to radiative recombinations of photoexcited holes essentially created in the region between the GaAs(buffer layer)/InGaAs interface and the doping-spike. Our results will be qualitatively explained considering the shape of the potential profile of the heterostructure which was obtained by solving the Poisson's equation by taking into account the Fermi-level pinning at the GaAs cap layer surface and residual doping due to the MBE growth conditions.

NEW RESULTS ON BOUND EXCITONS IN QUANTUM WELLS

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Excitons confined in semiconductor quantum wells have attracted much attention, particularly in regard to the influence of defects on the optical properties [1]. Recently Srinivas and co-workers discussed the bound exciton (BE) formation induced by above-barrier excitation due to defects localized at barriers [2]. In this work, we report photoluminescence (PL) and photoluminescence excitation (PLE) results obtained at 2 K in a conventional manner. The sample studied consists of 20-period GaAs/Ga_{0.7}Al_{0.3}As multiple quantum wells, grown by molecular beam epitaxy, where the wells and barriers are 80 and 300 Å wide, respectively. The PL spectra show a peak 1.2 meV lower in energy, relatively the free-exciton (FE) peak. From the PL and PLE results we eliminated bi-excitons, spin split due exchange interaction and monolayer fluctuations as the origin of this low-energy peak and associated it with bound exciton (BE) emissions. A line shape analysis supports this interpretation [3]. On the other hand, from the PL obtained with different excitation energies, a monotonous increase is observed in the BE peak intensity, relatively the FE peak. The BE peak become predominant for higher excitation energies due the carrier and capture mechanisms. The deconvolutions of the PL spectra show the unambiguous presence of the BE peak for excitation energy below the barrier. From the results we concluded, differently from the authors of reference 2, that the excitons are bound to ionized centers localized at interfaces.

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**SPECTROSCOPY OF OPTICAL PHONONS IN STRAINED GaSb/AlSb
SUPERLATTICES**

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Both Raman scattering and infrared spectroscopy were used to study the influence of strain and interface roughnesses on optical phonons in the GaSb/AlSb superlattices (SL's). The SL's have been grown by MBE on GaAs substrates. A 0.3 μm thick AlAs buffer layer was used to prevent the formation of defects in the SL's. The optical phonon lines originating from the AlSb buffer were found in the infrared reflection spectra. Their positions indicated that the strain in the buffer is almost completely relaxed. The comparison between the frequencies of the optical phonons confined in the AlSb layers revealed in the Raman spectra together with those of the unstrained AlSb buffer layer gave us a direct information about the strain in the AlSb layers.

It was found that the strain relaxes partially at the interface alloy intermixture regions. This strain relaxation depends on the thickness of layers, being stronger in those SL's which have thinner layers.

RAMAN ANALYSIS OF ALLOYING EFFECTS ON CRITICAL LAYER THICKNESS

IN $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ STRAINED HETEROSTRUCTURES

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Abstract

Raman scattering has been used to analyse the alloying effect on strain relaxation and to estimate the critical layer thickness in $\text{In}_x\text{Ga}_{1-x}\text{As}$ layers grown by molecular beam epitaxy on $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ [001]-oriented substrate for x ranging from 0.0 to 1.0. Measurements of LO GaAs-like phonon frequency and Raman linewidth showed that the indium/gallium ratio contents greatly influences the strain relaxation. The results can be explained in terms of the combined effect of strain and chemical and structural disorder.

ELECTRONIC STRUCTURE OF HOLES IN MODULATION DOPED
 $p-Si_{1-x}Ge_x/Si$ STRAINED QUANTUM WELLS IN A MAGNETIC FIELD.

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Recent growth of high quality $Si_{1-x}Ge_x/Si$ heterostructures has generated renewed interest in Si based quantum semiconductor nanostructures. The good quality of the interfaces between Si and Ge , when compared to those of the oxide-semiconductor, has led to samples of much higher mobilities. The combination of valence band mixing and strain, controlled by the Ge content, adds additional freedom in obtaining the desired electronic properties. The understanding of the properties of these materials requires the knowledge of these effects as well as of the properties of many interacting valence holes.

In this work the results of selfconsistent calculations of hole energy levels in strained, symmetric and asymmetric, p-type modulation doped $Si_{1-x}Ge_x/Si$ quantum wells in a magnetic field are reported. The band mixing is responsible for the enhanced effective g-factor of the opposite parity states. This leads to gaps at predominantly odd filling factors. The calculated filling factor dependent energy gaps are compared with gaps obtained from magneto-transport measurements.

Phase diagram for large two dimensional bipolarons in a magnetic field

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We perform a path-integral calculation of the ground state energy of a bipolaron confined to two dimensions and which is placed in a perpendicular magnetic field. The present calculation is valid for arbitrary magnetic field strength, arbitrary strength of the repulsion between the electrons, and arbitrary electron-phonon coupling constant. We find that the *bipolaron* exhibits: 1) a discontinuous transition from the polaronic state to the bipolaronic state, and 2) also exhibits a transition from the dressed state to the stripped state. These three transitions depend on the magnetic field and the strength of the repulsion between the electrons.

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DEPOPULATION OF ELECTRONIC SUBBANDS INDUCED BY A PARALLEL MAGNETIC FIELD IN AN ASYMMETRICAL QUANTUM WELL

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It is well known, at least theoretically, that a magnetic field applied parallel to the layers of an asymmetric semiconductor quantum well should depopulate the higher energy electronic subbands^{1,2}. The effect is due to two cooperative processes: firstly, the magnetic field increases the electronic effective mass, which leads to an increase in the density of states of the subbands, and, secondly, the diamagnetic shift gives rise to a decrease of the Fermi level relative to the subbands. Experimentally the effect has been little investigated since, due to the weak dependence of the electronic depopulation on the magnetic field, one needs high fields ($B \geq 10$ T) and specially fabricated samples in which the Fermi level is just above a high energy subband.

We study the effect of a parallel magnetic field, up to 17 T, on the optical and electrical transport properties of a quasi-two dimensional electron gas confined in a AlGaAs/InGaAs/GaAs asymmetric quantum well in which the first excited subband (e_2) is located only a few meV above the Fermi level. We show that the magnetoresistance and the photoluminescence intensity arising from band-to-band recombination of e_2 electrons have nearly identical dependence on the magnetic field, i.e., both are equally decreased as the field is increased. These observations can only be explained by the magnetic depopulation of e_2 . The dependence of the magnetoresistance on the temperature also confirms this interpretation. In addition, measurements in a similar sample which has the Fermi level just below e_2 do not show neither a negative magnetoresistance nor any decrease in photoluminescence intensities.

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STUDY OF MAGNETIC PROPERTIES OF SINGLE-ELECTRON QUANTUM WIRES SYSTEMS

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It is well known that the low dimension electronic devices are nowadays strongly investigated because of their large practical applications as well as its excellent theoretical framework in order to study the new behaviors of physics quantities in low dimensions systems. We have studied a system of single-electron confined in quantum wires and in presence of an external magnetic field. As first approximation we take an infinite harmonic oscillator potential to represent the wire and we do not include the electron spin, only the orbital contribution. The model Hamiltonian which has these two kinds of single-electron confinement was solved and with the eigenvalues, we performed a statistical-thermodynamics studies. The simplifications adopted in this model Hamiltonian allows us to obtain analytical expressions for the magnetic state equation and magnetic contribution to specific heat and entropy. The effect of temperature and the external magnetic field in z-potential-symmetry direction are fully discussed and proper analogies with metallic systems are presented. The results are shown in graphic way and the asymptotically region analyses are also performed.

**SEMICONDUCTOR FIBONACCI SUPERLATTICES:
ELECTRONIC AND OPTICAL PROPERTIES
IN THE PRESENCE OF A MAGNETIC FIELD.
SHALLOW IMPURITY STATES.**

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Abstract

A theoretical study of the magnetic sub-bands, electron wave functions, intraband and interband absorption spectra of GaAs-(Ga,Al)As quasiperiodic Fibonacci superlattices under in-plane magnetic fields, is presented. Calculations were carried out in the effective-mass approximation and parabolic model for both the conduction and valence bands were used. The attention is dedicated to the manifestations of the quasiperiodic, self-similar and anti-self-similar structural properties of these systems on the electronic and optical properties under study. The shallow impurity states in these superlattices are also calculated, and a theoretical study of the binding energy of these states is presented.

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RESONANT TUNNELING USED AS AN OPTICAL PROBE OF
ELECTRON AND HOLE DISPERSION CURVES OF A QUANTUM
WELL

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We have investigated the influence of an uniform electric field, applied in the growth direction, and an uniform magnetic field perpendicular to it, on the resonant tunneling of electrons and holes photogenerated in an asymmetric double quantum well system. To calculate the electronic structure of this system, we have developed a numerical technique based on the finite-difference and inverse power methods to solve the one-dimensional time-independent Schrödinger equation. The dispersion relations has been calculated for different values of electric and magnetic fields using the $\vec{k} \cdot \vec{p}$ mult-band model within a six-component envelope-function formalism. For a given value of electric field, i.e., for a given energy separation between the energy levels of the two quantum wells, we determine the magnetic field necessary to reach the tunneling condition. Hence, we obtain the electric *versus* resonant magnetic field curves and perform a systematic comparison between the electron and hole dispersion relations with recent experimental data. We have verified that for the analyzed heterostructure the in-plane magnetic field does not change appreciably the form of the hole dispersion curves, aside from a spin splitting of the hole states. Therefore, we find that the ground state of electrons (holes) localized in the narrow quantum well can be used as an optical probe for the dispersion curves of electrons (holes) states localized in the wide quantum well.

THE ROLE OF GRADED INTERFACES ON THE ACOUSTIC PHONON MODES OF Si/Ge SUPERLATTICES

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Recently, high-resolution transmission electron diffraction (HERTM) have shown the existence of graded interfaces in Si/Ge superlattices [1]. These graded interfaces can modify the vibrational properties of Si/Ge superlattices [2, 3]. The purpose of this work is to present a systematic study of graded interface effects on the energy mini-gaps at the edge and at the center of the Brillouin mini-zone. The nonabrupt Si/Ge superlattices are described by a linear chain model that takes into account the second neighbour interaction between the atomic planes. The graded $\text{Ge}_x\text{Si}_{1-x}$ interfacial alloy in the model are described through the virtual crystal approximation. The numerical solution of the dynamical equations shows that the gap splitting of the folded longitudinal acoustic modes are sensitive to the interface sharpness. The splitting gap of the second and third folded LA modes decreases with the growth of the interface width. The existence of interfacial asymmetry can change also the LA phonon frequencies. The results are in agreement with recent Raman experimental results [4], and with those obtained through a continuous model developed considering the space dependence of the $\text{Ge}_x\text{Si}_{1-x}$ alloy mass in the interface region [5].

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**IMPURITY EXCITED STATES IN GaAS LOW DIMENSIONAL
SYSTEMS UNDER APPLIED ELECTRIC FIELDS**

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Using a variational approach within the effective mass approximation we calculate the binding energy of some excited donor states in low dimensional systems with like-pill geometry, under the action of applied electric fields. We study the binding energy as a function of the geometry of the system, the applied electric field as well as the impurity position inside the structure. We found that in the quantum well, quantum-well wire and quantum dot limits of the like-pill geometry, our results are in good agreement with previous reports in those structures. Also, we found that the presence of the electric field breaks down the degeneracy of positioned symmetrical impurity excited states in these kind of structures.

Electronic properties of v-groove quantum wires structures

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We present a theoretical calculation of the electronic structure of v-groove quantum wires confined in modulation-doped n-AlGaAs/GaAs. The system investigated is sawtooth corrugated by bendings with period of 850 Å. The Schrödinger and Poisson equations are solved self-consistently. The method we use to calculate the electronic levels is based on the solution of the time-dependent Schrödinger equation using the split-operator technique. Results of the electronic structure are obtained as a function of the gate voltage and the donor impurity density. The electronic density shows the existence of a quasi one-dimensional electron gas.

SELF-CONSISTENT HOLE MINIBAND STRUCTURE CALCULATIONS OF ACCEPTOR δ -DOPING GaAs SUPERLATTICES

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The use of δ -doping in semiconductor materials has been demonstrated to be a powerful way of generating confined electron and hole gases of relatively high concentrations. While for n-type δ -doped layers in GaAs the energy miniband structures, potential profiles, Fermi level positions, minibands occupations, etc, are well known for a wide range of donor doping concentrations and superlattice periods, d , a detailed analysis of the energy band structure as a function of d and of the acceptor doping densities, N_A , is still lacking for p-type δ -doping GaAs. In this work we extend the self-consistent calculations of the hole band structure recently performed on p-type δ -doping GaAs superlattices [1] to include a wide range of parameters. The behavior of the hole minibands and their dispersion along k_z , the wavevector parallel to the superlattice axis, as a function of the superlattice period d and acceptor concentration N_A , is presented, covering from the isolated δ -well case to a superlattice regime. Concentrations are varied from 5×10^{12} to $1.5 \times 10^{13} \text{ cm}^{-2}$ and the periods range from 50 to 1000 Å. The calculations rely on the 4 X 4 Luttinger-Kohn Hamiltonian. To solve the corresponding multiband envelope function equation, a plane wave expansion is used. Many-body effects, such as exchange and correlation are taken into account within the local density functional approximation. It is shown that for periods d larger than 300 Å, the hole bands are practically dispersionless in the entire range of concentrations investigated. For a fixed period, the hole energy bands become deeper with the increase of N_A , as expected, since the δ -potential deepens. As d is decreased, the hole bands start to show some dispersion and a superlattice behavior takes over. For very short periods, $d \approx 50$ Å, the lowest hole bands are already relatively broad and partially overlap, being characteristic of strongly interacting wells. The transition from a twodimensional to a tridimensional hole gas is analysed. The results are compared with findings for the confined electron gas of n-type δ -doping wells in GaAs.

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Electron and hole states in lead-salt semiconductor heterostructures

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High quality semiconductor heterostructures with the peculiar family of lead-salts IV-VI compounds are now being grown by MBE. Here, the quantized states of electrons and holes confined in two, one and zero dimensions in lead-salt semiconductor quantum wells, wires and boxes, respectively, are studied within the standard envelope function approximation. Starting from the two-band (four with the spin) k - p Dimmock model for the bulk, we obtain analytical solutions for the quantized states originating from the different valleys, including both band anisotropy and non-parabolicity. The electronic subbands in PbTe/PbSnTe/PbTe quantum wells and quantum wires grown along both directions [111] and [100], with varying band offset, and the single-particle spectrum of infinity barrier square PbTe quantum boxes are calculated. Analytical solutions are also obtained in the case of structures without inversion symmetry showing strong spin-orbit splitting, which is linear in k both in the conduction and in the valence subbands. The band filling shift of the absorption edge at usual carrier concentrations is estimated and the its calculated dependence also on the well width and the band offset between these lead-salt compounds can help the determination of the latter with absorption measurements on different samples. The main qualitative differences between the spectrum of the IV-VI heterostructures with respect to that of the usual III-V structures are the almost specular symmetry between conduction and valence band and the multiplicity of the valleys oriented differently with respect to the growth direction.

ENERGY LEVEL SPLITTING IN DOPED NONABRUPT
 $\text{Al}_x\text{Ga}_{1-x}\text{As}$ DOUBLE QUANTUM WELLS

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RIT diodes based on double quantum wells - triple barriers have a better performance than those based on single quantum wells - double barriers. Multiple doped quantum wells are also important since they are the basis for semiconductor devices that operate at high currents. Interface regions with width of two and three unit cells were observed in multilayers $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ highly doped with Be ($\geq 10^{18} \text{ cm}^{-3}$) [1]. Recently, Freire *et al* [2] showed that interface and accumulation layers effects on the energy levels and carrier transmission of $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ heterojunctions are important in the case of high doping and large interfaces. The purpose of this work is to study the modification on the energy levels of doped $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ double quantum wells generated by the existence of graded interfaces. It is shown that the characteristic splitting of the energy levels is reduced considerably when interface widths of only two GaAs lattice units are taking into account. The interfaces also shift the energy levels towards high energies. Both the energy level splitting and shift depends on the level of doping.

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EXCHANGE INTERACTION OF DISORDER 2DEG ON THE SPIN-SPLITTED LANDAU LEVELS

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The Shubnikov-de Haas oscillations corresponding to the spin resolved Landau levels of 2DEG on $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ heterointerface were studied in the wide range of magnetic field (up to 22T) and tilt angle. The values of spin-splitting Δ_s were determined for half-filling Landau levels with Landau number $0\uparrow$ (spin up), $1\downarrow$ (spin-down), $1\uparrow$, $2\downarrow$ and $2\uparrow$ at wide range of the parallel component of the magnetic field. It was shown that using of the effective g-factor $g^* = \Delta_s / (\mu_B B_{\text{tot}})$ for characterization of the spin-splitting is not correct because the value of Δ_s depends on normal and parallel components of the magnetic field in a different and not a simple way. Analysis of these experimental dependences was made. The modification of the Zeeman spin-splitting by the exchange interaction of the electrons with different spin was taken into account in agreement with results obtained before. It is shown first that the broadening and overlapping of the neighboring Landau levels must be included into the spin-splitting treatment in real heterostructures. The overlapping of the levels with the same Landau number and different spins play the main role at small spin-splitting. For the case of large spin-splitting it is necessary to take into account the overlapping of the levels with different Landau numbers. The widely used coincident method was demonstrated not to give adequate results for g-factor and exchange interaction until Landau level overlapping is taken into account. On the basis of this model the experimental dependences of spin-splitting on magnetic field were described qualitatively and quantitatively. As a result the characteristic parameters spin-splitting such as the bare g-factor, the Landau level broadening and the value of the exchange energy were obtained for 2DEG in the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ heterostructure.

**DONOR-TYPE δ -DOPED CUBIC GaN SUPERLATTICES AND QUANTUM-
WELLS: MINIBAND STRUCTURE AND EFFECTIVE MASSES**

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The wide energy gap III-V nitride semiconductors, such as GaN, AlN, InN, and their related quantum-well heterostructures have received a great deal of attention for device applications in the blue and ultraviolet regions. Most of the studies in the III-nitrides has been concentrated on the wurtzite crystal phase. However, interest in zinc-blende cubic(c) nitrides has recently growing since they seem to be better suitable to produce controlled n- and p-type doped samples. The use of the δ -doping concept in III-V materials has been demonstrated, and shown to play an important role in the development of quantum electronic devices. With the recent advances also in the production of group-III nitride modulation doped heterojunctions and quantum wells, the investigation of δ -doping layers in GaN is highly desirable.

In the present work we report on self-consistent miniband structure calculation results of n-type δ -doped cubic (c)-GaN superlattices (SL) and quantum wells. The calculations are performed within the effective mass theory and the local density functional approximation for the exchange and correlation effects. The conduction band-edge effective mass of c-GaN, used to solve the one-dimensional Schroedinger and Poisson equations along the SL axis is obtained through an *ab initio* full potential Linear Augmented Plane Wave (LAPW) total energy calculation. Minibands, wave functions, energy dispersion relations along the wave vector perpendicular to the δ planes, and the corresponding miniband effective masses, are presented for several SL periods and different donor concentrations, covering the range from isolated δ -doped layers to a SL regime of highly interacting wells. Strong non-parabolicity of the miniband structure is observed. The perpendicular effective masses (along the SL axis) show a remarkable dependence on the kind of miniband, if confined or not by the δ potential wells. A comparison of the results with those obtained for other III-V compounds, e.g. GaAs is performed.

INTERFACE FORM BIREFRINGENCE IN (311)A GaAs/AlGaAs VERTICAL CAVITIES WITH NATIVE OXIDE

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We consider a novel form birefringence effect related to the formation of periodic corrugations in (311)A GaAs/AlGaAs interfaces. A simple model is proposed in which the corrugations are assumed to have a square-wave profile with alternating refraction index whose period is much smaller than the cavity mode wavelength.

We exploit the proposed effect in the context of cavities with few reflector pairs of large-index-step high contrast Bragg (DBR) mirrors, obtained by lateral oxidation of high Al composition layers of small mesa samples¹⁻³. A striking polarization selection of the cavity modes is achieved in this case (see Fig. 1), with potential use in polarization controlled emission of vertical cavity surface emitting lasers with very short cavities.

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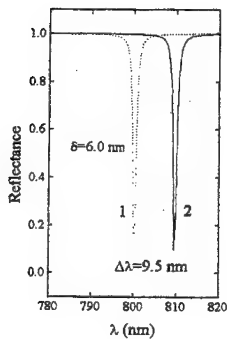


Fig. 1. Calculated reflectance spectra of a vertical λ -cavity whose upper and lower DBR mirrors consist of three GaAs/oxide pairs with large refractive-index ratio (3.5/1.6) with $\lambda=800$ nm. Curves 1 and 2 refer, respectively, to the cavity modes with electric field parallel and perpendicular to the corrugations. The width of the GaAs/oxide interface regions $\delta=6.0$ nm is considered in our calculations. The two cavity modes are separated enough ($\Delta\lambda=9.5$ nm) to ensure a polarization selected emission.

POSTER SESSION II

HOPPING CONDUCTION IN GaAs: δ (Si)

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The process of hopping conduction in a two-dimensional electron gas (2DEG) continues to attract much interest both experimentally and theoretically. In this work we report on electrical conduction via the hopping mechanism on a 2DEG in GaAs with silicon planar doping, GaAs: δ (Si). A single layer of Si impurities is incorporated in GaAs during the molecular beam epitaxy growth, with relatively low silicon doping concentrations ($N_{2D} \leq 1 \times 10^{12} \text{ cm}^{-2}$). The magnetic field and temperature dependence of the conductivity under illumination with below band-gap radiation show a change in the conduction regime from activated to metallic conduction. In the dark, the resistance dependence on temperature, the magnetoresistance and the Hall voltage dependence on magnetic field show characteristics of the hopping regime of conduction. After illumination, the electrical properties gradually change from hopping to metallic conduction. The concentration and mobility of the conduction electrons increase monotonically with illumination. This means that we can adjust the number of electrons that take part in the hopping process via the light dose that the sample has been submitted to.

We study the mechanisms of hopping conduction, in the insulator phase of the sample, for different degrees of illumination. Measurements of the resistivity as a function of temperature can be fitted by $\rho \propto \exp(T_0/T)^s$, where s is a parameter between zero and one. From these fits we can get information on the impurity density of states at the Fermi level, $g(\epsilon) \propto (\epsilon - \epsilon_F)^m$, where the exponent m is related to s . We follow the behavior of $g(\epsilon)$ and the exponent m with the increase in the number of hopping electrons (as the light dose is increased).

ELECTRON TRAPPING AND LIGHT INDUCED METASTABILITY IN N-TYPE SnO_2 THIN FILMS

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Tin dioxide is a wide bandgap ($\cong 3.5$ eV) oxide semiconductor. Its optical transparency and electrical conductivity make SnO_2 particularly attractive for transparent electrodes for many kinds of optoelectronic thin film devices. Thin films of pure, Sb-doped and Nb-doped SnO_2 have been prepared by sol-gel dip-coating technique on glass substrates. The amount of Sb or Nb doping (2%) leads to a expected highly degenerate n-type conduction. Measurements of resistance as a function of temperature show electron trapping which presents two ranges of capture. The first level, having a potential barrier of about 30 meV, can be related to scattering at grain boundary, while the other one of about 70 meV for the thermal activation energy, can be associated to a deep level, whose nature is under investigation, being probably a Sb complex. Monochromatic light excitation (305 nm) at low temperature induces a metastable increase in the sample conductivity, which can not be destroyed as the sample returns to room temperature. Three different metals have been evaporated for improving the electrical contact to SnO_2 samples : Cu, In and Au. The same metastable conductivity effect is obtained, no matter the evaporated contact or the annealing time and temperature, although a slight shift in resistivity is observed. This communication reports results of optical absorption, complex impedance, resistance as a function of temperature in the dark and under influence of monochromatic light. Electrical transport modeling and electron capture parameters are also presented. Based on these electro-optical characteristics, the potentiality of these films for optoelectronic devices are discussed.

CAPACITANCE SPECTROSCOPY OF INTERACTING VALENCE
HOLES IN P-SiGe DISKS IN A MAGNETIC FIELD.

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There is currently interest in SiGe based quantum confined semiconductor nanostructures, such as quantum disks, self-organized dots, and submicron tunneling diodes compatible with existing silicon technology. The SiGe systems differ from the well studied GaAs system in a number of ways. Unlike in GaAs, in SiGe based quantum wells the electrons are, at best, weakly confined and only valence band holes show significant quantum confinement effects. Since current technology allows for charging GaAs nanostructures with individual electrons, one might expect to study in near future strongly interacting holes in SiGe nanostructures as well.

In this work we study the interaction of holes in p-SiGe quantum disks in a magnetic field. The holes are described by a Luttinger Hamiltonian, with parity replacing spin as a good quantum number. The interaction Hamiltonian separates into charge-charge and parity-parity parts. The effect of parity mediated hole-hole interactions is illustrated by numerical calculations of the energy and capacitance spectra for two holes in a quantum disk for parameters corresponding to a SiGe system.

CAPACITANCE-VOLTAGE PROFILING OF PERIODICALLY Si- δ -DOPED SEMICONDUCTORS

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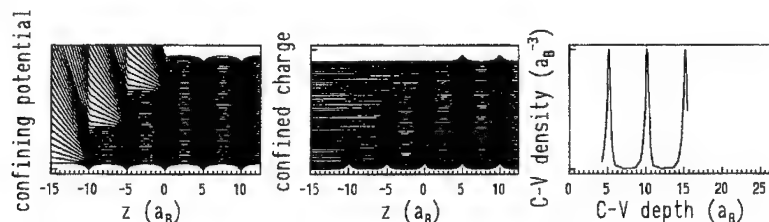
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Capacitance-voltage profiling (C-V) is an experimental technique which was originally devised to resolve the doping profile in the proximity of the heterojunction of two homogeneously doped semiconductors (see, for instance [1]). More recently, the C-V technique has been successfully used to resolve the doping profile in semiconductor systems with quantum-confined carriers [2]. Schubert showed that for a δ -doped semiconductor the C-V spectrum is described by a peak whose width at half-maximum is drastically dependent on the spatial localization of the dopants [2]. The characteristic width of the doped layer can be inferred with a precision of one or two monolayers by calculating the theoretical C-V profile (obtained from a self-consistent solution of Schrödinger and Poisson equations for the structure under bias), whereby the doped layer width is an input parameter.

In this work we extend the C-V spectrum analysis to *periodically* δ -doped semiconductors. The C-V spectrum was measured for periodically Si δ -doped InP, and oscillations are seen whose period are very nearly equal to the intended doping period. The C-V spectrum was calculated, and oscillations are also seen, and it is demonstrated that the period of oscillations can be taken as an accurate measure of the doping periodicity (see Figure below). The effects of temperature, doping level and period, and density of background impurities upon the theoretical C-V spectrum are studied and discussed. The theoretical analysis allows one to establish practical limitations of the C-V technique when applied to periodically delta-doped semiconductors.



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THE INFLUENCE OF CYCLOTRON FREQUENCY ON ELECTRON TUNNELLING ACROSS $GaAs/Al_xGa_{1-x}As$ MULTIPLE BARRIERS

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When an electron tunnels through a simple $GaAs/Al_xGa_{1-x}As$ heterojunction barrier submitted to a magnetic field perpendicular to the growth axis, the circular component of its motion in the direction perpendicular to the growth axis and whose radius is related to the cyclotron frequency, is important and can modify certain tunnelling characteristics. In the work presented here, we have studied the influence of cyclotron frequency on electron tunnelling across $GaAs/Al_xGa_{1-x}As$ multiple barriers submitted to a magnetic field perpendicular to the growth direction of these barriers. We also present numerical results obtained by solving the Schroedinger equation using the multistep method. We show that the cyclotron frequency causes electron transmission resonance peaks to shift towards high energy. The resonance peak shifts increase with increasing applied magnetic field intensity, though these shifts are only significant when the applied field is greater than 10T. These shifts also depend on the number of heterostructure barriers.

We have studied simple $GaAs/Al_xGa_{1-x}As$ barriers of 50Å and 100Å wide. No considerably effect was observed in electron transmission across the 50Å well when submitted to magnetic fields less than or equal to 30T. Only small changes were observed for the case of the 100Å well. We have also investigated simple abrupt barriers of 100Å with interface width of 2 GaAs lattice parameters (LP) when submitted to magnetic fields of 0T, 10T, 20T and 30T. We observed that the influence of the interface is more important than that of the applied magnetic field.

Magnetic fields of up to 30T were applied to a double barrier of 100Å wide, with interface width of 2 LP and a quantum well of 100Å wide. We have also studied the presence of interfaces of 1 LP, 2 LP and 4 LP and observed that an interface width of 2 LP is critical to the modification of transmission properties across $GaAs/Al_xGa_{1-x}As$ double barriers.

In the case of multiple barriers, the change in the electron tunnelling characteristics does not depend only on the modifications of the potential barrier height produced by the applied field, but also on the alterations produced by the quantum well energy levels that the electrons use when tunnelling. The energy level modifications are of the order of 10meV for quantum wells of 100Å wide and applied magnetic field of about 10T.

UNIVERSAL DIAGONAL AND HALL CONDUCTANCE FLUCTUATIONS IN A RANDOM MAGNETIC FIELD.

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The localization problem for a two-dimensional electron gas (2DEG) experiencing a random magnetic field has recently attracted considerable interest, in large part due to its relevance for the fractional Hall effects. Quantum interference effects are responsible for the localization at zero magnetic field. In small, mesoscopic samples quantum interference leads to the sample specific universal conductance fluctuations (UCF), which have an amplitude of the order of e^2/h . It has been predicted, that in a random magnetic field the amplitude of UCF is still of the order of the universal value, although the correlation properties will depend on the specific realization of the random potential. We have studied diagonal and Hall conductance fluctuations in a mesoscopic 2DEG grown on substrates with prepatterned, submicrometer dimples. When placed in magnetic field B parallel to the substrate, the electrons in such system move in sign-alternating, random B [1]. We find UCF in parallel external magnetic field with amplitude in order of e^2/h , however, the correlation properties of these fluctuations in a random magnetic field are governed by the second order corrections to the flux through the closed electron trajectories. We tested global symmetry relations for both diagonal and Hall conductance fluctuations. We have found that fluctuations of the antisymmetric part of the Hall conductance $\Delta\sigma_{xy}^a = (\Delta\sigma_{xy}(B) - \Delta\sigma_{yx}(B))/2$, extracted by interchanging of current and voltage leads, are not equal to fluctuations of Hall conductance, extracting by changing of B sign: $\Delta\sigma_{xy}^a = (\Delta\sigma_{xy}(B) - \Delta\sigma_{xy}(-B))/2$. Thus, $\Delta\sigma_{xy}(B) \neq \Delta\sigma_{yx}(-B)$, and Onsager relation is violated in such system in contrast to diagonal resistance, for which $\Delta\sigma_{xx}(B) = \Delta\sigma_{yy}(-B)$. We also found that the amplitude of $\delta\sigma_{xy}^a$ is in order of e^2/h in a random magnetic field as predicted by perturbation theory [2] and numerical calculation of the Chern numbers in a mesoscopic conductor [3].

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MAPPING THE ELECTRONIC WAVE FUNCTIONS BY DETERMINING CURRENT X VOLTAGE CURVES

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Resonant tunneling in double barrier heterostructures in the presence of impurity planes is studied within the Green function formalism following the diagram technique for nonequilibrium processes proposed by Keldysh¹. A simple one-band tight binding Hamiltonian is adopted in the theoretical framework. Electronic densities of states are obtained for different 3-dimensional heterostructure configurations. Characteristic curves of current versus voltage, concerning with transport properties in double and triple barrier systems evidenciate the evolution of the quasi-bound states in the quantum-well regions. The effects of an isoelectronic impurity plane, localized in the well region of a GaAs- GaAlAs double barrier heterostructure, on the resonant curves of the current are analyzed as a function of the impurity plane position. The theoretical results suggest that the evolution of the bias corresponding to the first and second resonant peaks are quite close to the spatial variation of the associated electronic wave function. Experimental probing of quantum-well eigenstates was previously reported by Marzin et al² who used planar isoelectronic perturbation to measure, by typical photoluminescence experiment, the spatial dependence of the probability density associated with a discrete set of eigenstates. Our theoretical results for the resonant bias indicate unambiguously that, besides optical measurements, transport experiments can be performed for the mapping of the wave functions in quantum-well systems.

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MEASUREMENT OF THE HEAVY AND LIGHT HOLE MASS IN InGaAs/InAlAs QUANTUM WELLS

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The prediction of optical transition energies with accuracy is of critical importance for the design of opto-electronic devices. For quantum-well devices using ternary and quaternary semiconductors, this is severely hampered by large uncertainties in the anisotropic hole masses. We report new experimental results that should greatly improve our ability to make accurate predictions. Photocurrent measurements at 10K with different reverse biases on lattice matched InGaAs/InAlAs multiple quantum wells (MQW) with different well widths ($w=70\text{\AA}$, 85\AA and 100\AA) have been performed. By extrapolating the bias dependent energy positions of all the observed transitions to zero field and by comparing with detailed numerical simulations, we obtain accurate values of perpendicular and parallel heavy-hole and light-hole masses.

**EXPERIMENTAL OBSERVATION OF PHOTOINDUCED ASYMMETRIC-
DOUBLE-WELLS COUPLING IN MODULATION DOPED
HETEROSTRUCTURES**

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Using a combination of magnetotransport techniques we have assessed the population of the electron states in silicon planar-doped AlGaAs/GaAs heterojunction grown by MBE. The change in the subband populations were induced by illuminating the samples with an infrared LED. We have created the conditions for a resonance-induced delocalization of two states which, far from resonance condition, are located either in the planar doping region or at the interface. The quantum resonance was directly observed as a region of negative differential resistivity for both the photoconductivity curve as a function of the light dosage and in the photoconductivity curve as a function of temperature in a heating experiment after illumination. In conclusion, we have observed experimentally the quantum resonance induced by photo excitation and by thermal regeneration.

THE BOHM-AHARONOV AND KONDO EFFECTS ON TUNNELING CURRENTS IN A MESOSCOPIC RING

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We present an analysis of the Kondo effect on the Bohm-Aharonov oscillations of the tunneling currents in a mesoscopic ring with a quantum dot inserted in one of its arms. The ring is threaded by a magnetic flux and the dot is subjected to a gate potential. The system is described by an Anderson-impurity tight-binding Hamiltonian where the electron-electron interaction is restricted to the dot. The currents are obtained using non-equilibrium Green functions calculated through a cumulant diagrammatic expansion in the chain approximation.

We investigate the current going along the quantum dot in two different situations: at low temperature when the system is in the Kondo regime and at high temperature when the flowing charges are dominated by the resonant tunneling condition. At low temperature the Kondo peak provides a channel for the electron to tunnel through the dot and we obtain Bohm-Aharonov oscillations of the current even if the system is out of resonance. At high temperature these oscillations appear only if the dot level is aligned to the Fermi level.

THE ROLE OF DOPING ON THE ULTRAFAST TRANSPORT TRANSIENT IN p-GaAs AND n-GaAs

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The understanding of the dynamics and high field transport of carriers in heavily doped semiconductors is relevant for the design improvement of high-speed bipolar and heterojunction bipolar transistors. High doping has important effects on the carrier dynamics and transport properties in semiconductors. Experimental results showed that the energy dissipation rate [1] and the mobility [2] of hot minority carriers in p-GaAs increase with doping. Monte Carlo simulations have highlighted the effect of the electron-hole interaction on the steady-state transport [3] and on the ultrafast relaxation of hot minority carriers in p-GaAs as a function of doping. In particular, Alencar *et al* [4] showed that a reduction in the overshoot effect in p-GaAs related to the electron-hole interaction is obtained when the doping increases. In this theoretical work, a comparison is made between the role of doping on the ultrafast transport transient of minority and majority carriers in p-GaAs and n-GaAs, respectively. During the evolution towards the steady-state, both the drift velocity and temperature of the majority carriers are shown to be higher than those of the minority carriers. This is true for all the electric field intensities and level of doping. When the electric field intensity is lower than 8 kV/cm , the drift velocity of minority and majority carriers have the same time evolution pattern up to a doping density of $1 \times 10^{19} \text{ cm}^{-3}$. If the electric field intensity is higher than 8 kV/cm , it is shown that an increase of the doping can preclude the existence of an overshoot effect in the drift velocity of the minority carriers, but not in the drift velocity of the majority carriers.

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ELECTRON HEATING EFFECTS IN A FREE STANDING WIRE OBSERVED BY UNIVERSAL CONDUCTANCE FLUCTUATIONS

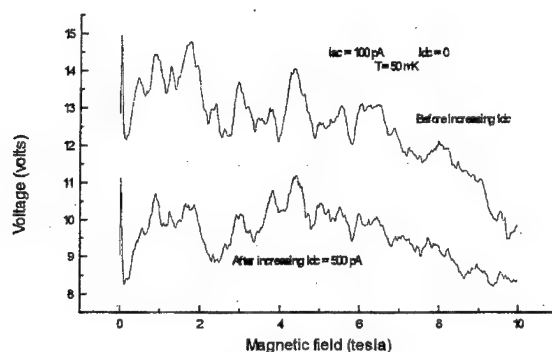
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In this work we have intentionally employed a series of free standing wires in order to study the effect of a DC current in Universal Conductance Fluctuations. Free standing wires offers the possibility of studying local heating up effects on the electron interference due to the increase of temperature at centre of the wire. The structure was preliminary created by growing a two dimensional electron gas in a GaAs/AlGaAs heterostructure. Devices were fabricated at centre of a Hall bar using electronic lithography and deep wet etching. Several free standing wires were produced with length 1-10 μm and width 0.5-1 μm . Measurements were performed at temperatures of sample T_s down to 50 mK and magnetic fields up to 10 Tesla. We have done a set of experiments where DC injected current I_{DC} was added to AC locked one. Universal Conductance Fluctuations were measured as function of magnetic field, T_s and I_{DC} . The correlation functions of different $I \times B$ curves will be presented and it is possible to extract the local region where heating up is more effective. Results sign the possibility of using injection current across wires to change impurity configuration specifically at centre of such devices, due to localised heating up effects.



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**Effect of Terahertz Induced High Population of the First Excited State
on the Electric Transport of a Multi-Quantum Well Superlattice**

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We used a free electron laser (FEL) to resonantly induce intersubband transitions between the two first levels of a multi-quantum well (MQW) superlattice, increasing dramatically the population of the second level (near the saturation). The power necessary to do so is much smaller than the necessary to observe photon-assisted tunneling without intersubband transition. We observed an increase of the conductivity of the sample around zero bias, a decrease of the current at the bias region between the two first plateaus, and a new plateau over the second plateau of the IV characteristic. The resonant frequency of these three effects and the relation with the bias where they happen is measured and analyzed.

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**THE EFFECT OF HIGH LANDAU SUBBAND FILLING
ON HOT-ELECTRON MAGNETO-TRANSPORT
TRANSIENT IN InSb**

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Hot-electron high-magnetic field transport in semiconductors is an interesting research subject because both the high electric field and the Landau quantization of the energy band have to be taken into account simultaneously. The effect of high Landau subbands filling on the steady-state properties of hot electrons is important in InSb subjected to high electric and magnetic fields (\vec{E}/\vec{E}). [1] The theoretically calculated electron drift velocity in InSb exhibits negative differential mobility for magnetic field intensities up to 25 T if the occupation of only the lowest Landau subband (the extreme-quantum-limit) is assumed. However, the negative differential mobility is precluded when the filling of all the possible Landau subbands is considered. This work is concerned with the effect of high Landau subband filling on the ultrafast hot-electron magneto-transport transient in InSb. Two coupled differential equations for the electron energy and drift velocity are solved in the approximation of momentum and energy relaxation times. [2] It is shown that the electron drift velocity and temperature are considerably overestimated if their calculations are based on the extreme-quantum-limit assumption. In the case of $E = 2.5 \text{ kV/cm}$ and $B = 2 \text{ T}$, the drift velocity overshoot calculated under the extreme-quantum-limit assumption is about two times larger than that obtained by taking the filling of all possible high Landau subbands into account.

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STUDY OF THE PROPERTIES OF THE IMPURITY BAND OF $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}:\text{Si}$ WITH DIFFERENT ELECTRON CONCENTRATIONS.

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A doped semiconductor with doping concentration lower than a typical critical value is an electrical insulator. At temperatures lower enough to inhibit thermal activation of carriers to the conduction band its electrical conduction occurs in the impurity band. Several models have been proposed to explain the behavior of the conductivity in the impurity band¹. The main mechanism for compensated doping consists of thermal assisted tunneling of carriers from occupied to unoccupied impurity sites. This mechanism is called *hopping* and encompass several models. All of them predict a temperature dependence of the conductivity like $\sigma \sim \exp(T_0/T)^p$. The p value depends on the model and is related with the behavior of the density of states at the Fermi level. It has been found that each model may apply to a specific regime of temperature depending on the carrier concentration. So the models are not incompatible one with each other.

We have done experiments on a single sample of the $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ alloy Si doped with an approximate concentration of $6.8 \times 10^{17} \text{ cm}^{-3}$. The concentration of electrons in the shallow impurity band was changed from $7 \times 10^{15} \text{ cm}^{-3}$ to $1.3 \times 10^{17} \text{ cm}^{-3}$ by light incidence which transforms the deep level Si into shallow donor. Above $1.7 \times 10^{17} \text{ cm}^{-3}$ the sample seems to become metallic. The temperature was varied from 0.35 to 60 K. Our setup was able to measure resistance as high as 200 G Ω . The resistivity versus temperature was obtained for 27 different electron concentrations. The results show clearly the $p = 1/2$ behavior proposed by Efros and Shklovskii in a wide band of temperatures and electron concentrations. For several concentrations one can see also another regime at temperatures lower than those of the $p = 1/2$ behavior. It was not possible to decide whether this regime is related to a hard gap² in the density of states ($p=1$). For some electron concentrations it seems even that two $p = 1/2$ regimes, with different values of the T_0 parameter, would fit better the data. All the data was then fitted with a variable p . The values of p are related to the shape of the density of states at the Fermi level. In this way the density of states for the impurity band could be analyzed for all the electron concentrations.

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BLOCH OSCILLATIONS VIA BOLTZMANN TRANSPORT FORMALISM

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We derive the Bloch oscillating currents in a semiconductor superlattice from a Boltzmann transport equation approach, in the relaxation time approximation. We have incorporated in the calculations the whole band structure of a superlattice. The zero temperature time dependent current obtained when a constant uniform electric field F is applied along the superlattice axis has two contributions: a) a large transient current which clearly shows oscillations at the Bloch frequency eFd/h , where d is the superlattice period, and b) an initially smaller, out of phase oscillating current which eventually becomes the non zero steady state contribution. Depending on the magnitude of the electric field, the steady state component may be an order of magnitude smaller than the initial amplitude of the oscillating current. The current-voltage characteristics of the steady state component recovers the well known negative differential conductivity as initially established by Esaki and Tsu.

**ELECTRIC-FIELD EFFECTS ON THE SPIN RELAXATION OF
ELECTRONS IN *p*-DOPED GaAs QUANTUM WELLS**

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We study the effects of an applied longitudinal electric field on the spin-relaxation rate of electrons in *p*-doped GaAs/Al_xGa_{1-x}As quantum wells. The spin-relaxation mechanism investigated derives from the electron-hole exchange interaction, which is particularly sensible to the applied electric field since it depends directly on the wave-function overlap of the electrons and holes. The eigenstates of the system, for the conduction and valence bands, are calculated self-consistently following the Split-Operator method in semiconductors. This calculation is capable of describing a wide range of semiconductor heterostructures. The spin-flip rates are obtained by the electron-hole scattering, via the exchange interaction, in the Born approximation. We show that the electron spin-relaxation time is very sensible to the longitudinal electric field due to two adding effects. First, increasing the electric field the electron and hole states separate apart, decreasing the exchange strength and lengthening the spin-relaxation times. Second, with still increasing fields, holes are removed from the quantum well, which also contributes to a slower spin relaxation. Similar dependence on the electric field is not expected in the electron spin relaxation by other mechanisms relying on the spin-orbit interaction. Therefore, this effect can be used to determine the relative importance of the different spin-relaxation mechanisms in a systematic experimental study of the luminescence polarization emitted by *p*-doped GaAs quantum wells.

QUANTUM CORRECTIONS TO THE CONDUCTIVITY DUE TO WEAK ANTILOCALIZATION IN THE ASYMMETRIC INGAAS/INP HETEROSTRUCTURES.

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The magnetoresistivity measurements were made on the selectively-doped $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ heterostructures with 2DEG at very low magnetic field (2–100 G). For the samples with 2DEG density from $2 \cdot 10^{11}$ up to $2 \cdot 10^{12} \text{ cm}^{-2}$ the magnetoconductivity is the nonmonotonic function of the magnetic field (so called "antilocalization minimum"). This is evidence of the significant role of the spin-orbit interactions in the electron-wave-function interference. Description of the experimental results was made using both commonly accepted theory of Hikami et al [1] and modern theory [2]. The last one takes into account in spin-splitting both terms that are cubic and linear in electron-wave-vector, which arise due to the lack of inversion center in the crystal (Dresselhaus terms), as well as additional linear term which concerned with the asymmetry of the quantum well (Rashba term). The following results were obtained for the samples, in which 2DEG occupy only one subband:

- * the temperature and resistivity dependences of the phase relaxation rate are in a good agreement with the theory of the electron-electron interaction with small momentum transfer;
- * linear terms in spin-splitting have to be taken into account to describe experimental results;
- * the density dependence of the spin-orbit rate demonstrates that the Rashba term dominates in the spin-orbit relaxation; the comparison of experiment results and theory allowed us to determine spin-splitting parameters of 2D electrons in the asymmetric $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ quantum wells.

The following results were obtained for the samples, in which electrons occupy two subbands:

- * the antilocalization minimum in magnetic dependence of the magnetoconductivity dramatically decreases with the appearance of carriers in the second subband;
- * the comparison with theory showed that the occupation of the second subband leads to the rise of the effective rate of the phase relaxation, but at the same time the effective spin-orbit relaxation rate decreases. We attribute such behaviour of these effective rates not only with the difference of the diffusion coefficient of carriers, but also with the difference between characteristic relaxation times of electrons in the first and second subbands. The supposed model permits us to describe experimental dependences qualitatively.

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InGaAs/AlGaInAs/InP laser with compressively strained MQW layers for high speed modulation bandwidth

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Strained multiquantum (MQW) layers are very attractive in high performance distributed feedback (DFB) semiconductor laser devices for applications in high speed and long distance optical communications. In the present work, high frequency response measurements are presented for DFB lasers comprising a separate confinement heterostructure (SCH) with MQW layers of InGaAs/AlGaInAs/InP emitting at 1.55 μ m wavelength. The SCH-MQW layer structure was grown by MBE and incorporates 10 compressively strained (1.2%) InGaAs QW layers 30Å thick between AlGaInAs lattice matched barrier layers (emission wavelength 1.26 μ m) 80Å thick. The waveguiding layers were designed asymmetrically in order to reduce the difference in transport distance between holes and electrons and thus, maximize the differential gain ($\delta g/\delta n$). The DFB grating was defined on the upper AlGaInAs layer with a negative detuning from the maximum of the gain spectrum. The lasers were processed with the mushroom-stripe structure, which presents a low parasitic capacitance for high speed performance (1). The frequency response measurements were undertaken using the small signal analysis technique and employing the logarithmic subtraction of the parasitic electric response of the laser device (2). A high value of $\delta g/\delta n = 8.73 \times 10^{-16} \text{ cm}^2$ was obtained with a low damping K factor coefficient of 0.21 nsec. The frequency modulation bandwidth measured for the laser devices was around 20 GHz.

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STUDY OF GaAs: δ -Si ETCHING RATES BY ATOMIC FORCE MICROSCOPY

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It is known that the morphology of metallic layers grown on semiconductor surfaces depends on the semiconductor doping profile [1]. In addition, a previous work by Sá de Freitas *et al.* [2] indicated that the etching rate of GaAs: δ -Si could be dependent on the distance of the planar doping layer from the surface. These results are only two examples of the influence of the bulk doping profile of a semiconductor on its surface properties. In particular, it is clear the importance of the GaAs: δ -Si etching rate for the design and fabrication of semiconductor devices. In this work, we present a systematic study of the etching rate of GaAs as a function of the distance of a Si-doped planar layer from the surface. The work was carried out using atomic force microscopy to monitor the etching process on different samples of GaAs: δ -Si grown on (100)-oriented substrates and it is shown that the GaAs etching rate decreases as the surface-planar doping layer separation decreases. Different etching agents and substrate orientations were also investigated during this work. A phenomenological theory, considering surface adsorption and oxidation mechanisms, is used to model the experimental results.

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SULFUR PASSIVATION OF GaAs IN ALCOHOLIC SOLUTIONS.

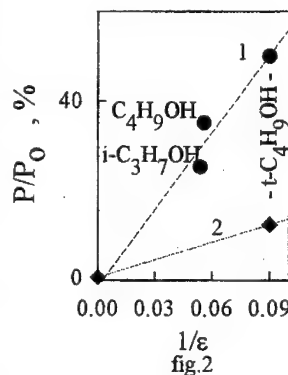
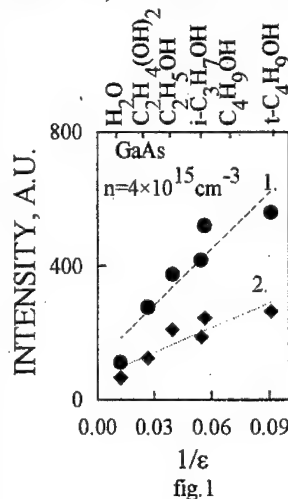
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Photoluminescence and x-ray photoelectron spectroscopy were used to show that the effectiveness of passivation of GaAs surface electronic states could be increased considerably by the use of the Na_2S -solutions or $(\text{NH}_4)_2\text{S}$ -solutions in which alcohols with low dielectric constant (isopropanol, tert-butanol etc) are used as solvents.

It has been found that with the decrease of the solvent dielectric constant in such solutions the surface sulfur coverage increases, the thickness of the native oxide layer decreases, and the efficiency of band-edge photoluminescence increases (for Na_2S -solutions - curve 1, fig.1). The same dependences occur after GaAs passivation in the alcohol-based $(\text{NH}_4)_2\text{S}$ -solutions but to a lesser extent (curve 2, fig.1). It's allows to propose a new method - sulfur passivation in alcoholic solutions [1]. This method has been applied for facet passivation of InGaAs/AlGaAs SQW laser diodes [2]. It has been shown that such treatment results in the increase of the lasers slope efficiency and catastrophic optical damage level. The value of the increase of the catastrophic optical damage level depends on the solution dielectric constant as well as the efficiency of GaAs passivation. This increase is the highest (50%) when Na_2S -t- $\text{C}_4\text{H}_9\text{OH}$ -solution with the lowest dielectric constant was used (curve 1, fig.2). It has been found that the same dependence occurs after facet passivation in $(\text{NH}_4)_2\text{S}$ -t- $\text{C}_4\text{H}_9\text{OH}$ -solution (curve 2, fig.2) but to a lesser extent (only 15%).

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**DYNAMICS OF (100) InP SURFACES: EFFECT OF SURFACE STEPS ON
EQUILIBRIUM SHAPE AND NUCLEATION**

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Understanding the morphology of grown films has become an important issue in the last few years, due to the knowledge on basic physical processes and also to its application in the creation of new heterostructures. In this work we report a study by Atomic Force Microscopy (AFM) on the equilibrium morphology of (100) InP surfaces as a function of substrate miscut in different directions, and its effect on the nucleation of thin InP homoepitaxial films by Chemical Beam Epitaxy. In order to analyze the evolution of the surface toward its equilibrium shape, the substrates were annealed at 530°C under P₂ overpressure for different time intervals. Thin (5 and 10nm) InP films were deposited on the annealed substrates. The growth conditions used determined whether the growth mode was two or three-dimensional.

The AFM shows that the evolution of the surface during annealing depends strongly on the surface miscut. After an initial rearrangement of the steps on the surface due to the miscut, different morphologies are observed for substrates with nominal orientation or 2° off presenting mainly A, B or both (A and B) type of steps (respectively, A, B and C surfaces). For the nominal substrate the terraces - with small two-dimensional islands on top - become wider as annealing time increases. For the A, B and C surfaces, however, structures with larger height variation begin to form on the surface. For the A-surface, mainly the morphology is affected by this process, with roughness kept nearly constant with annealing time. For B and C surfaces, however, morphology and roughness change due to annealing. Multiterrace structures - slightly elongated along the [011] direction - form on the surface, indicating a stronger interaction between B-type steps.

We then observe the nucleation of InP films on the annealed surfaces. The deposited films had a minimum thickness of 5nm, larger than the peak-to-valley height variation in the annealed substrates. For growth conditions where the film grows on a three-dimensional mode, no significant changes were observed in morphology when different substrates or annealing times were used. For films deposited in a two-dimensional growth mode, however, different behaviors were observed. Planarization of the surface was achieved at 5nm only for nominal and A-surfaces. The B and C surfaces present morphologies with larger structures, in lateral dimensions and height, than the initial substrate. The structures increase in size as growth proceeds, showing a smaller micro and larger macro-roughness as the thickness of the layer is increased to 10nm. This behavior is explained by the presence of an energy barrier at B-step edges which minimizes the interlayer transport required to planarize the surface.

ATOMIC STRUCTURE CALCULATIONS OF THE CUBIC GaN (110), (100) AND (111) SURFACES

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The recent advances in the fabrication of GaN based blue light and UV-emitting diodes and lasers diodes have generated intense interest in the properties of the wide band-gap group III nitrides. Most of the electronic and optoelectronic devices that have been successfully built so far are based on the wurtzite phase of these materials grown on sapphire substrates. However, the metastable zinc-blende phase (β -GaN) is expected to be more suited to efficient n- and p-type dopings, following the properties of other III-V semiconductor compounds. This fact motivated successful attempts to grow high quality β -GaN films on GaAs, Si and β -SiC substrates, and prompted several authors to study their properties. In this work we have carried out self-consistent tight-binding total energy calculations of the β -GaN (110), (100) and (111) surfaces. These studies pave the way to the understanding of the growth processes of GaN and of the physical properties of heterointerfaces between this material and other group III nitrides and substrates. The GaN surfaces are represented within the framework of a 96 atoms-slab model comprising 2×4 supercells extending over twelve monolayers. By calculating the total energy of a supercell as a function of the atomic positions, we search for the minimum energy which defines the stable atomic configurations for the surface. We conclude that the (110) surface does not reconstruct but relaxes leading to calculated bond angles in fairly good agreement with ab initio cluster model calculations.¹ For the Ga-terminated polar (100) surface the Ga atoms do not dimerize, unlike the N-terminated surface where the N atoms form dimers with a bond length of about 1.40 Å.² As far as the Ga-terminated (111) surface is concerned, 2×4 supercells with π -bonding for N-terminated surfaces, and without such bonding for Ga-terminated surfaces. All models are very close in total energy, and in all cases the displacements of atoms are almost perpendicular to the surface, this implies that relaxation rather than reconstruction takes place within these models, independent of surface termination. The situation changes if the formation of vacancies is allowed at the surface. Removing 2 of the 8 supercell atoms of a Ga-terminated surface, then total energy is considerably lowered, and the reconstruction becomes 2×2 . Similar calculations for the N-terminated surface are in progress.

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INITIAL OXIDATION OF THE HYDROGENATED Si <111> SURFACE

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The Si/SiO₂ interface is surely one of the most studied in the field of semiconductors, because of its fundamental role for device physics. A number of models have been proposed for the structure of the transition region, which is known to be of very complex nature. It is also speculated that the final structure may have a memory of the growth process; thus, the initial stages of surface oxidation are of special interest, and merited extensive experimental investigations. Theoretical studies, on the other hand, are specially difficult because one must focus on isolated surface defects, which would demand unusually large supercells. We present a study of the hydrogenated Si <111> surface, under atomic Oxygen exposure. We find that the subsurface interstitial site is preferred for O absorption, and that clustering, or island formation, is highly favored. To be able to perform this investigation, we simulate the surface through a molecular cluster model (clusters with 50 and 134 atoms), including four Si layers, and terminated on the back side and lateral boundaries with Si pseudoatoms. We use a semiempirical parametrization of the Hartree-Fock method, MNDO/Crystal, that allows us to obtain self-consistent charge densities, total energies and vibrational frequencies. We study the incorporation of subsurface interstitial O, isolated and in clusters of up to 3 atoms, thus reaching the saturation limit of the back bonds of a Si-H unit. We allow relaxation of the top layers (H and 3 Si), in the case of the free Si-H surface; the defect is then placed at the center of the surface, and allowed to relax (including first and second neighbors). We obtain Si-H stretching frequencies within a few percent of the experimental values, and find a shift to higher energies with the number of O atoms that supports the experimental assignment. Total energy calculations indicate a gain of the order of 1-3 eV per atom for the clustering, which clearly indicates that island formation should dominate the initial stages of oxidation of this particular surface.

A STUDY OF METAL-SiC INTERFACES

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The interface between metal and silicon carbide presents a wide range of electrical (Schottky and ohmic contacts) and structural properties. In the latest years experimental work has shown that, at room temperatures, the reactivity of most metals (Pd, Au, Co, Ti, Ag, Al) is, in general, small; in addition these interfaces present a significant range of ϕ_B , the Schottky barrier. More recently it was shown that the interface properties can change with temperature. The interest in wide band gap semiconductor materials that could be effective in high temperature, motivates the great amount of experimental and theoretical work in these systems.

We use the extended Hückel approximation to study electronic of the β -SiC interface with different metals. The COOP (Crystal Orbital Overlap Population), aside from the band structure and DOS (Density of States) analysis will be used as an attempt to establish trends of behavior, e.g., the changes in metal-surface bond for different metals. Our aim is the understanding of simple and basic mechanisms of electronic interaction at the interface.

Structure and Energetic of GaAs:Te and InAs:Te Surfaces*

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We have carried out ab-initio total-energy density-functional calculations to examine the reconstruction and surface energies of GaAs(001)(2x2):Te and InAs(001)(2x2):Te surfaces as a function of Te surface coverage. The reconstructed surfaces consisting of various combinations of dimers and Te coverage were determined. Our calculations indicate that a full monolayer of As ($\theta_{\text{Te}} = 0$) is energetically more favourable than any of the studied coverage of Te ($\theta_{\text{Te}} = 1/4, 1/2, 3/4, 1$), where the stability is reduced with increasing Te coverage. The surface's As atoms dimerize around 30% more than surface's Te atoms. Comparing the Te dimerization on InAs(001)(2x2):Te, In terminated, and GaAs(001)(2x2):Te, Ga terminated, we observed that the Te atoms dimerize 40% more over InAs than GaAs. Another observation is the tendency of the Te atoms to "float" from the surface with increasing coverage: from 0.10Å ($\theta_{\text{Te}} = 1/4$) to 0.25Å ($\theta_{\text{Te}} = 1$). For any Te concentration we verify that there is almost no interaction between the (-110) chains on both structures that could increase the surface free-energy. Finally our results show that for the same concentrations of Te the atoms prefer to be adsorbed on the sites off-chain indicating a monoatomic adsorption.

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**STUDY OF GaSb AND AlSb SURFACE SUPERSTRUCTURE
BASED ON THE (100) PLANES**

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Surface superstructure (SS) on semiconductor surfaces determines properties like Schottky barrier heights, vacancy densities and surface adatom migration length at the molecular beam epitaxy (MBE). In this work we have studied the evolution of surface structures as function of the substrate temperature on the (100) AlSb and GaSb by RHEED analysis. Atomic smooth surfaces were produced by MBE on the (100) GaAs substrates. As the temperature of the Sb-rich surfaces of AlSb and GaSb increases from the room temperature, it is observed that the surface superstructure is changed to the (4x2) metal stabilized one. On the GaSb (100) surfaces were observed the following number of SS: the (2x5)Sb-stabilized, (1x3) and (2x4)Ga stabilized SS. The phase transition from the (2x5)Sb-stabilized SS to (1x3) ones goes through unusual changing of superstructure strike positions. This can be explained considering the SS rotation during the phase transition relatively to the bulk lattice. The strike intensities for different azimuths of the (2x5) SS are altered in a factor 2, indicating a lower SS ordering across the domain axe (x2). On the AlSb surfaces the following SS sequence were detected: at low temperature there is a superposition of the (6x1) and (2x1) SS, at higher temperatures (3x1), (3x3) and (2x4)Al-stabilized structures. We have supposed that the low temperature SS (6x1)+(2x1) have more than one monolayer coverage by Sb. We have also observed for the first time evidences of mixed surface superstructures (6x1)+(2x1) and SS (3x3).

ADHESION OF THE CVD DIAMOND FILM DEPOSITED ON Ti6Al4V ALLOY IN VARIOUS TEMPERATURES

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The extensive use of titanium and its alloys is based primarily on two very important characteristics: high strength-to-weight ratio and excellent corrosion resistance. Titanium's strength-to-weight ratio has made it a basic structural material for aircraft and aerospace applications. Ti6Al4V alloy is specially used in prosthesis of multiple uses due to its bio-compatibility. However, this alloy has low wear resistance. So, the addition of a thin CVD diamond film can give an extended life to this material for specific applications. In this work, CVD diamond films were deposited on Ti6Al4V alloy by hot filament technique considering different substrate temperature and deposition time. First of all, an enhanced diamond nucleation was obtained using 0,25 μ m diamond powder suspension in n-hexane in ultrasonic bath. It was observed better adhesion of thin diamond film on Ti6Al4V substrate surface at lower temperature. We speculate these results come from the alloy phase transformation. In high temperature this effect is more apparent. In order to overcome this barrier some experiments in the limit of low temperature growth conditions was performed. In addition, the mechanical properties of the alloy were partially recovered using a dehydrogenation procedure. At these conditions, after 12 hours of deposition time a 5 μ m thick diamond film appear with good adhesion on titanium alloy. The quality and morphology of the film was obtained by Raman Scattering and SEM analysis. The surface modifications concerning diamond deposition conditions were analyzed by EDX.

Formation of Si-c/ β FeSi₂/Fe-c Structure by Two Step Annealing and Ion Beam Mixing in Fe Thin Film and Si Substrate

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β FeSi₂ is a direct gap semiconductor with 0.85 eV in forbidden band, and candidate to optical communication laser source (1.54 μ m wavelenght) in Si technology.

Fe thin film were deposited in highly clean $\langle 111 \rangle$ orientation Si substrate in a Balzer evaporation system. In order to promote the reaction the samples were submitted to two steps thermal annealing cycles in high vacuum or irradiated with Xe⁺ at the energy of 380 keV with doses ranging from $2.0 \times 10^{15} \text{ cm}^{-2}$ to $2.0 \times 10^{16} \text{ cm}^{-2}$.

Employing a two step thermal annealing procedure (e.g., 200/350°C + 420/500°C) it is produced a structure composed of a layer of β FeSi₂ interposed between the Si substrate and the oriented crystalline Fe film. The Xe⁺ irradiation conducted with samples held at room temperature leads to a mixed layer at the Fe/Si interface with the β -FeSi₂ the most abundant phase. If the sample is submitted to thermal annealing after irradiation the mixed layer is completely converted to β FeSi₂. The samples were analysed by Rutherford Backscattering Spectrometry (RBS), Conversion Electron Mössbauer Spectroscopy (CEMS) and X Ray Diffraction.

HIGH RESISTIVITY SILICON LAYERS OBTAINED BY HYDROGEN ION IMPLANTATION

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This work presents a study of the perspectives of the use of hydrogen ion implantation in silicon as option to obtain a superficial stable crystalline layer electrically isolated from the silicon substrate. The scope of this work is to obtain an improved quality surface region over a damaged high resistive buried layer. High resistive layers are obtained by hydrogen ion implantation on p doped (100) Czochralski silicon wafers with resistivity equal to $14 \Omega \text{ cm}$.

The implantation energy used was 100 KeV and doses ranging from $2.0 \text{ E}14 \text{ H}^+/\text{cm}^2$ to $2.0 \text{ E}16 \text{ H}^+/\text{cm}^2$. After the implantation the wafers are submitted to a 900°C by a Rapid Thermal Annealing (RTA) up to 64 s and by Conventional Thermal Annealing (CTA) to 1200°C up to 100 minutes. After the thermal process, it was verified the permanence of the high resistivity buried layer. Spreading resistance profiles show resistivity peak values around $300 \Omega \text{ cm}$ at $1.0 \mu\text{m}$ below the surface.

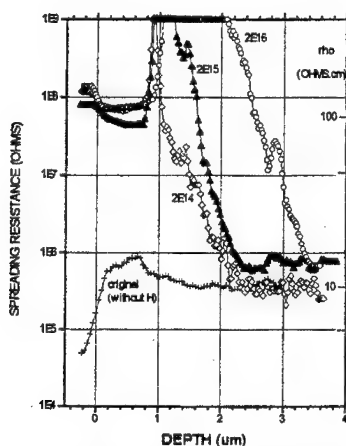


Fig. 1: Spreading resistance profiles for hydrogen implanted samples with 100 KeV and doses: $2\text{E}14$, $2\text{E}15$ and $2\text{E}16 \text{ H}^+/\text{cm}^2$

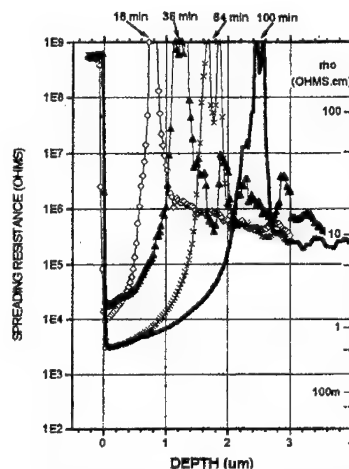


Fig. 2: Spreading Resistance profiles for hydrogen implanted samples (100 KeV, $5\text{E}15 \text{ H}^+/\text{cm}^2$) followed by RTA (900°C , 64s) and CTA (1200°C and indicated times)

**THE ELECTRON-PHONON INTERACTION IN SEMICONDUCTOR
FILMS WITH INTERFACIAL DELTA DOPING**

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The understanding of the surface properties of thin semiconductor films is a matter of relevance to the development of technological applications. The electron-phonon coupling in semiconductor systems is a very important subject [1]. In particular, polaronic states were shown to be present in semiconductor slabs [2]. Recently, delta-like charge confinement are generating new interesting phenomena [3]. The purpose of this work is to investigate the effect of a delta-like charge density at both surfaces of a semiconductor slab on the properties of confined electrons. Maxwell equations are solved with appropriate boundary conditions to obtain the dispersion relations of surface plasmons. They are used to obtain the second quantized Hamiltonian that describes the coupled electron-phonon system in the semiconductor film. Numerical results are obtained for the dispersion relation and the electron-phonon coupling function for GaAs. It is shown that the delta doping does not change the volume modes, but alter significantly its surface modes. The delta doping effects on the electron-phonon coupling function depend either on the surface charge density, as well as on the film thickness, and increase with the reduction of the slab width.

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RENUCLEATION STUDIES ON CVD DIAMOND FREE STANDING FILM

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CVD diamond as thin and free standing film presents the most important and convenient advantage in comparison with HPHT and natural diamond in term of application field, that is the almost unlimited substrate surface shape. Besides the surface shape, low roughness is necessary for optical and/or tribological applications. For abrading application high roughness is required. So, in this work studies involving renucleation process on CVD diamond surface in contrast to columnar structure as a function of some growth parameters was performed. It was observed a strong dependence of the renucleation density in several steps of diamond coating as a function of the gas flow rate and carbon contents. Renucleation process is more accentuated when very low gases flow rate is used during the CVD diamond film deposition, while the columnar structure is dominant when high flow rate is used. We speculate that when very low amount of precursors' gases is present in the diamond growth process the columnar structure is interrupted. We identified a minimum flow rate for renucleation onset. Also, the growth rate in renucleation state is lower than in columnar growth state. Morphological phenomena and quality measurements of the CVD diamond film surfaces were figured out by SEM, x-ray and Raman Scattering Spectroscopy.

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ELECTRONIC STATES OF THE INTERFACE $\text{CuInSe}_2 / \text{CdS}$

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In this work, results will be reported concerning the calculation of the density of electronic states in the $\text{CuInSe}_2 / \text{CdS}$ interface. This results are of technological significance, because, up to date, the best thin film solar cells have been fabricated using the $\text{Cu}(\text{In,Ga})\text{Se}_2$ heterostructure.

The tight binding method was used for the calculations; the Hamiltonians were calculated with s and p orbitals for indium, selenium, cadmium and sulfur and s , p and d orbital for copper. It was assumed an ideal interface without reconstructions and without stretching. The interface was built using the (112) surface for the CuInSe_2 and the (001) surface for the CdS . The tight-binding parameters for the interface were calculated using the Harrison's formulae.

The Density of States (DOS) and the dispersion relations (E versus k in the 2-dimensional Brillouin zone) were calculated from the Green's function using the transfer matrix method. The results indicated the presence of energy states in the gap of both CdS and CuInSe_2 . The influence of the band offsets of the $\text{CdS}/\text{CuInSe}_2$ system on the interface states was also investigated.

OPTICAL SPIN POLARIZATION IN N-TYPE MODULATION-DOPED QUANTUM WELL

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We present optical polarization measurements in a n-type one-side modulation-doped single quantum well (QW). We study the carrier spin polarization in a sample under Hydrogen passivation and compare the results with those for the as-grown sample.

Optical measurements using circular polarized light give information about the spin relaxation of photocreated carriers in semiconductor QW. In doped semiconductor QW the main contribution to the optical polarization is given by the minority carrier. In previous work¹, we presented the continuous-wave (CW) optical polarization in a n-type one-side modulation-doped AlGaAs/InGaAs/GaAs QW. In this sample the electron gas density is $2 \times 10^{12} \text{ cm}^{-2}$ and the Fermi level is just above the second conduction subband. We observed that the electrons close to the Fermi level partially conserve their spin polarization. In this case, the electrons that are photocreated close to the second subband edge have a small wave vector. Under this situation, the electron spin relaxation mechanisms² are less efficient and one observes the electron spin polarization.

In this work we compare these results with those obtained in the same sample after Hydrogen passivation. The Hydrogen atoms neutralize the donors in the AlGaAs layer diminishing the transference of electrons into the InGaAs QW. After passivation the electron density decreased from $2 \times 10^{12} \text{ cm}^{-2}$ to $1.4 \times 10^{12} \text{ cm}^{-2}$. Only the first conduction subband is occupied and no electron spin polarization is observed in the vicinity of the Fermi level. In this case, the electrons are only photocreated with large wave vector. The electron spin relaxation is more efficient and no electron spin polarization is observed in the CW regime.

¹ Triques A.L.C. et al, Superlattices and Microstructures, 1996 in press.

² Maialle M. Z., Phys. Rev. **B54**, 1967 (1996).

INTERFACE ROUGHNESS STUDIES IN DOUBLE BARRIER STRUCTURES

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Photoluminescence spectroscopy is used to investigate tunneling of electrons and holes through GaAs/In_{0.1}Ga_{0.9}As/AlAs double barrier tunneling structure with interface roughness. Typical quantum well photoluminescence spectra present a splitting attributed to interface roughness effects, namely growth island formation in the quantum well. The position, intensity and linewidth of these lines are investigated as function of applied bias and temperature. The integrated photoluminescence intensity and linewidth of both lines are correlated to tunnel current bias in the low photoexcitation intensity. A transfer of carrier between these islands is observed at the beginning of resonant tunneling regime. Near the resonant peak, this transfer is reduced since both islands are almost equally populated by electrons in the resonant tunneling process. Finally, the states of these islands are selectively populated by electrons and holes with applied bias.

2.5 GBIT/S, LOW-CHIRP, DIRECTLY-MODULATED FIBRE GRATING LASER FOR OPTICAL NETWORKS

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Abstract: Very low wavelength chirp (static < 0.04 GHz/mA and dynamic < 0.1 GHz/mA) is reported for a directly modulated fibre grating laser with an angled facet semiconductor chip. We report on transmission achieved at 2.5 Gbit/s over 300 km of standard and $> 10,000$ km of dispersion shifted fibre.

The laser consists of a $450\text{ }\mu\text{m}$ GaInAsP/InP buried heterostructure amplifier chip with an angled facet coupled to a lensed fibre grating with a peak reflectivity of $\sim 60\%$ and a FWHM reflection bandwidth of 0.19 nm . The angled facet amplifier chip has a very low front facet reflectivity of $< 5 \times 10^{-4}$. The effective length of the external resonator was measured to be $\sim 4\text{ mm}$. The laser operated stably on a single longitudinal mode with a side-mode suppression ratio $> 45\text{ dB}$ and low relative intensity noise $< -145\text{ dB/Hz}$. The laser linewidth was less than 0.4 MHz at the output power of 1 mW . The static wavelength chirp was determined from the spectral position of the dominant and suppressed (spontaneous background) modes at different dc currents (above threshold) to be $< 0.04\text{ GHz/mA}$. The dynamic wavelength chirp was obtained from the time resolved measurements of the laser spectra when the FGL was directly modulated by 2.5 Gbit/s PRBS signal ($I_{\text{mod}} = 30\text{ mA}$; 40 mA) and DC bias current $I_{\text{dc}} = 1.4 I_{\text{th}}$. The observed chirp in the FGL spectra is less than 0.04 nm (resolution limited) when 40 mA of modulation signal is applied.

The FGL was modulated at 2.5 Gbit/s with an NRZ PRBS ($2^{15}-1$) pattern in a recirculating fibre loop consisting of an optical amplifier and $\sim 35\text{ km}$ of dispersion shifted (Corning DS) or $\sim 39\text{ km}$ of standard (Corning SMF-28) fibre. Zero power penalty due to dispersion in SMF was measured up to 117 km . BER of $\leq 10^{-9}$ was measured for distances up to 270 km , with some degradation over 300 km . The measured BER shows penalty-free transmission over 1100 km of DS fibre. Single channel transmission results over longer distances will be discussed at the conference.

SCATTERING RATES IN A SEMICONDUCTOR HETEROSTRUCTURE.
THE ELECTRON-PHONON COUPLING

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We present a rigorous application of the physics of continuous media (including the corresponding matching problem) to describe polar optical oscillations in a semiconductor heterostructure which is modeled as follows: a semi-infinite slab of a semiconductor material having an interface with another semiconductor with its second surface free. The polar optical phonons (POP) for this system are analyzed in detail and an analytical expression for the electric potential generated by the oscillations in the unretarded limit ($c \rightarrow \infty$) is obtained. We also derive the Frölich-like Electron-POP hamiltonian for this case. The obtained hamiltonian is applied to the calculation of Scattering Rates assuming the zero-temperature limit, when only the POP emission is possible. We consider the case of intra-subband transitions, assuming complete electron confinement within the active layer and representing the electronic states by a linear combination of Airy functions. A detailed discussion of the results is made.

OPTICAL SPECTRA OF QUASI-PERIODIC SEMICONDUCTOR SUPERLATTICE

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Although the electronic properties of semiconductor superlattices and multi-quantum-wells have attracted enormous attention in the last decade, considerably less effort has been done on the optical properties of these artificial specimens. In particular, these properties in a new class of artificial crystal, the so-called quasi-periodic structures, seem to have important interesting features. These quasi-crystals are formed by the superposition of two (or more) incommensurate periods, so that they can be defined as intermediate systems between a periodic crystal and the random amorphous solids. On the other hand, the propagation of light in quasi-periodic layered materials could provide an excellent way to probe experimentally localized states. The reason for that is because localization phenomenon is essentially due to the wave nature of the electronic states, and thus could be found in any wave phenomena.

It is the aim of this work to present the optical spectra of multiple layers in a quasi-periodic arrangement forming a Cantor set. Using a transfer matrix approach, to simplify the algebra which is otherwise much involved, we find the reflectance and transmission theoretical expressions for quasi-periodic structures which obey the Fibonacci, Thue-Morse and Double-period substitutional sequences. Then, we present numerical calculations of these spectra which show, among other interesting properties, a rich structure of self-similarity, with a series of scaling point in the reflection (and transmission) pattern, physically characterized by a dip (peak) of the reflectance (transmission) spectrum. Of course, these scale points form themselves another Cantor set. A comparison with the spectra found in periodic structure is also done, with more interesting features to understand the physical properties of these quasi-periodic structures.

**PHOTOLUMINESCENCE SPECTRA ASSOCIATED TO SHALLOW
ACCEPTORS IN $\text{GaAs-Ga}_{1-x}\text{Al}_x\text{As}$ QUANTUM DOTS**

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A systematic study of the theoretical acceptor-related photoluminescence spectra in a spherical $\text{GaAs-Ga}_{1-x}\text{Al}_x\text{As}$ quantum dot is performed. The acceptor states are described within a variational scheme in the effective-mass approximation considering an finite-confinement model. Photoluminescence spectra associated with acceptors are calculated for homogeneous doped distributions of acceptors in the quantum dot. The interaction between the impurities has been neglected. The main features found were two peaks associated with transitions involving impurities close to the center and at the edge of the quantum dot, which modify their intensities depending on the temperature, and the size of the dot. We compare our results with those found in quantum wells and quantum-well wires of comparable dimensions.

PHOTOREFLECTANCE AND REFLECTANCE STUDY OF GaAs/GaAlAs-BASED HEMT DEVICES

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Recently, semiconductor device structures have been studied by means of photoreflectance (PR) spectroscopy. In this work we present an experimental and theoretical PR study of high electron mobility transistor (HEMT) structures. As in previous investigations, we find two types of oscillations, one type with large period, which can be interpreted in terms of the Franz-Keldysh effect, and another type with short period whose origin is controversial at present. One possible origin of this type of oscillations are optical transitions from the valence band to the 2D electron states of the HEMT. To check the validity of this interpretation we performed PR measurements in the presence of a gate voltage, which allows us to change the position of the Fermi level with respect of the quantum well (QW) bottom. This should result in a shift of the short period oscillations if they actually were due to the 2D electron gas of the HEMT. No shifts were observed however, proving that the origin of the short period oscillations is not related with the 2D electron states. The new interpretation we propose here relies on the existence of an interface charge at the active buffer layer / substrate interface. This interface charge gives rise to an electric field, sufficiently strong to create Franz-Keldysh oscillations but essentially smaller than the surface field, explaining the shorter period of these oscillations. Calculations of the field profile and PR responses following this line of interpretation result in PR spectra which are in very good agreement with the experimental results. The fitting of calculated and measured unmodulated reflectance spectra was used to accurately determine the layer thicknesses of the structures.

STRUCTURAL AND PHOTOLUMINESCENCE CHARACTERIZATION OF POROUS SILICON WITH RAMAN SCATTERING SPECTRA

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Raman Scattering has become a powerful tool to study the characteristic dimensions of silicon crystallites in porous silicon layer. The analysis is based mainly on the phonon confinement model in which the finite crystallite size is taken into account by the weighting wave function of phonon in crystal silicon. Smaller silicon crystallite leads to a red shift and broadening of the phonon Raman spectra [1,2].

Results obtained with Raman Spectroscopy are used to estimate the crystallite size and correlate it with the photoluminescent behavior of the porous silicon layer.

Porous silicon layer was obtained from Boron doped (100) silicon of 20 Ωcm resistivity with HF 48% (w/o) aqueous solution at current density of 20 mA/cm^2 .

The Raman spectra were obtained on a Renishaw Raman system 3000 equipped with a CCD detector. The measurements were made in the back scattering geometry using a microscope objective for focusing the laser beam. The data reported here were obtained at room temperature. The laser source was the 632.8nm line of HeNe laser from spectra physics. The laser power at the samples was less than 70 μW . The spectral resolution is 1 cm^{-1} .

The LO Raman Scattering spectra obtained from porous silicon led us to estimate three crystallite sizes: 3.0 nm, 4.0 nm and 11.0 nm. The photoluminescent spectra of these structures shifted to the blue as the crystallite size decreased.

Crystallite size around 2.96 nm, 2.98 nm, 3.10 nm are calculated based on the quantum confinement model used to explain the photoluminescence phenomena.

The difference observed between crystallite size using Raman Scattering and photoluminescence spectra can be justified because of the assumption of a ideal quantum confinement model.

[1] Campbell I. H and Fauchet P. M.; "The Effects of Microcrystal Size and Shape on the One Phonon Raman Spectra of Crystalline Semiconductor". Solid State Comm. V 58, N 10, pp. 739.

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OPTICAL CHARACTERIZATION OF CARBON NITRIDE THIN FILMS

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Carbon nitride thin films are produced by the ion and vapor deposition method. The films are formed by carbon evaporation by an electron beam with simultaneous nitrogen ion bombardment on Si(100) and fused silica substrates. The ion beam energies for film formation are 0.5, 0.8, 2.0, 5.0 and 10.0 keV and the composition ratio C/N varies from 0.4 to 3.0. X-ray induced photoelectron and Fourier transform infrared spectroscopy are used to study the bonding state and to estimate the composition ratio between carbon and nitrogen. X-ray diffraction patterns show that the films are amorphous or contain undetectable crystallites. Spectrophotometry in the visible and ultraviolet regions are used to study the transmittance and optical density. The transmittance spectra show dependence on the energy of the ions and on the composition ratio C/N. The optical band gap is calculated from the optical absorption spectra by the Tauc formula. The optical band gap shows a strong dependence on the composition ratio C/N and on the ion energy. For samples prepared at low ion energy and low composition ratio a band gap up to 2.7 eV is obtained.

(This work is partially supported by CNPQ, FAPESP and FINEP)

**OPTICAL CHARACTERIZATION OF $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$ LAYERS
BY INFRARED TRANSMISSION**

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The samples have been grown on (111) cleaved BaF_2 substrates by Molecular Beam Epitaxy at temperatures between 200 and 300 °C. The growth was "in situ" monitored by a 10 keV Reflection High Energy Electron Diffraction system. The Sn content of each sample has been determined by x-ray diffraction, assuming that the lattice constant varies linearly with alloy composition. The electrical properties have been addressed by resistivity and Hall effect measurements at temperatures from 13 to 350 K.

A Fourier Transform Infrared Spectrophotometer has been used for measuring the transmission at wavelengths from 2.2 to 22 μm at temperatures between 77 and 300 K. The experimental results have been fitted using a two-band **K.p** model including the effects of the non-parabolic energy bands and uses only four fitting parameters: energy gap, oscillator strength, lifetime broadening and background index of refraction.

From the fittings, the dispersion of refraction index and absorption coefficient and their dependence with temperature have been derived below and above the energy. For the samples with high Sn content, the observed energy gap was much higher than the value expected from the literature. This is an effect of the high carrier concentration, which produces a Burstein-Moss shift of the energy gap in these samples. The optical parameters obtained for these single layers can be used in the determination of the optical properties of multi-quantum well structures made with these materials, using the same fitting procedure. Preliminary results for one multi-quantum well sample consisting of 50 repetitions of $\text{PbTe}/\text{Pb}_{0.85}\text{Sn}_{0.15}\text{Te}$ will be reported.

**BIDIMENSIONAL DIFFUSION INVESTIGATION USING
PHOTOLUMINESCENCE IMAGING IN InGaAs-InP QUANTUM WELLS**

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We have used a new spectroscopic technique based on the imaging of photoluminescent regions of optically excited quantum wells to study transport in these samples. This technique presents advantages over other conventional techniques for not requiring the use of electrical contacts or a special growth geometry of samples to measure the diffusion length and the local density of carriers. We then propose to scan the photoluminescence image and to measure the local spectrally integrated photoluminescence intensity on the surface of the samples. The samples are VLE grown InGaAs/InP quantum wells whose 2D diffusion can be investigated since the spatial distribution of carriers depends on radiative recombination mechanisms. We use a spectrometer to show the photoluminescence spectra at different sites on the sample surface spaced radially from the center of the laser spot. We then compare the photoluminescence spectra from sites where carrier density is high with those far from the center, where the density is low.

PHOTON-ASSISTED TUNNELING STUDIES IN A DOUBLE BARRIER DIODE

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We have measured $I(V)$ characteristic and photoluminescence spectra of double barrier diode with roughness interface and island formation in the quantum well under high photoexcitation intensity. We have observed a reduction of the resonant peak, peak to valley ratio and bistability region in the $I(V)$ characteristic due to the change of electronic charge stored in the well induced by photon absorption and emission process. The photoluminescence spectra under high photoexcitation intensity are measured as a function of applied bias and temperature. We have observed a correlation between quantum well integrated photoluminescence and tunnel current for the highest energy peak. A saturation is observed for the lowest energy peak which reduces the transfer of carriers between islands in the tunneling process. Another interesting effect is the marked correlation between linewidth and tunnel current for both peaks under high photoexcitation intensity which is controlled by Fermi energy in the quantum well and by the degree of hole localization and disorder in the system.

RADIATIVE AND NON-RADIATIVE RECOMBINATION IN QUANTUM-WELL WIRES

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Abstract

A quantum-mechanical calculation and phenomenological treatment of radiative and non-radiative recombinations respectively in $GaAs$ - $(Ga, Al)As$ quantum-well wires, excited by a cw laser in a photoluminescence experiment under quasistationary excitation conditions, considering different densities of shallow and deep impurities, are performed. In the case of shallow impurities, we work within the effective-mass approximation and the parabolic-band model for describing both electrons and holes, and consider, in the steady state, the interband absorption, and some radiative recombination mechanisms, such as recombination of electrons with free holes and with holes bound at acceptors. The effects of deep impurities (traps) are studied at room temperature of phenomenological form where of the nonradiative rates associated with transitions involving electrons falling into traps, and trapped electrons recombining with free holes. Carrier densities, chemical potentials, and electron-hole recombination decay times are calculated as functions of the temperature and laser intensity. Theoretical results in the case of shallow impurities are in good agreement with available experimental data.

ENHANCED NONLINEAR OPTICAL RESPONSE FROM A STEEP AND GENTLY SLOPING SURFACE RELIEF: WHAT IS THE DIFFERENCE?

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The enhancement of nonlinear optical susceptibilities of composite materials having different mesoscopic geometries was predicted and recently observed experimentally for a composite of alternating sub-wavelength-thick layered structure¹. Here we calculate the effective second-order nonlinear susceptibility $\chi^{(2)}$ of else one simple structure: low relief interface between linear medium and the material with second-order nonlinearity. We obtained analytical solutions for the cases of steep and gently sloping low relief elongated periodical irregularities. Both the lowness and the periodicity are essential for receiving of exact solutions.

Consider the periodical relief. The procedure of solving this problem is analogous to going over from microscopic to macroscopic Maxwell's equations in a medium. The details of the particular structure of the relief do not affect the characteristics of the reflected radiation. The reflection is only influenced by a certain limited amount information about the relief. Spatially nonuniform fields, which depend on the shape of the relief, vary over distances comparable to the length scales of the relief, its period and its height. Since these distances are much shorter than the wavelength, the quasistatic approximation is sufficient for calculating the "microfields". In that approximation, however, the fields satisfy the Laplace equation, and their spatially varying part is known to fall off exponentially with distance from the interface. The minimum rate of this decay is comparable to the reciprocal dimensions of the relief. Only spatially uniform fields "survive" outside a narrow surface layer. And since wave zone begins at distances from the surface which are comparable to the wavelength, where the microfields have decayed, the relief and its shape affect the scattering only through the average fields. These physical arguments lead to the following mathematical formulation of the problem. Let us introduce layer which thickness is much larger than the period l and height h of the irregularities, but much smaller than the wavelength λ of the incident radiation. It is sufficient to solve the static problem in this layer, where the spatial averages of the field and the displacement vector satisfy the relation

$$\langle D \rangle = \hat{\epsilon}^{eff} \langle E \rangle \quad (1)$$

where tensor $\hat{\epsilon}^{eff}$ is the local tensor, in accordance with the approximation $\max h, l / \lambda \ll 1$. If one medium have the nonlinear susceptibility $\chi_0^{(2)}$ and linear permittivity ϵ_0 , whereas other medium may be linear with the permittivity ϵ , then the electric field amplitude become concentrated in the more nonlinear medium in a surface layer, resulting in enhancement overall effective response of the surface. For the trench form of the irregularities the most enhanced is χ_{xxx} component of the effective nonlinear tensor and for the triangular form of the irregularities the most enhanced are χ_{xxz} and χ_{zzz} components.

1. George L.Fischer et al, Phys.rev.Lett. 74, 1871 (1995).

Exciton-bound electron spin relaxation

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Exciton luminescence polarization studies in semiconductor quantum wells have revealed the coexistence of two main mechanisms of exciton spin relaxation. A well known direct relaxation with simultaneous electron and hole spin flip due to the electron-hole exchange interaction and an indirect one via the optical non-active states with sequential spin flip of the single particles. The exciton spin relaxation time in this indirect channel is determined by the lowest single particle spin-flip rate, which is in general the electron one. In the present study the exciton-bound electron spin dynamics driven by the spin-orbit interaction in the conduction band is discussed. The off-diagonal matrix element in the space of the pairs of optical active and inactive exciton states, that differ only with regard to the electron spin direction, represents the effective magnetic field, that changes randomly as the exciton is elastically scattered and relaxes its spin. The exchange splitting between the optical active and inactive states acts as an external magnetic field, reducing the relaxation. The estimated rate of the bound electron spin flip agrees well with values obtained from previous fittings of the experimental data. The well width and temperature dependence of such exciton spin relaxation mechanism, which becomes the most important one in the case of real space indirect excitons, are also briefly discussed.

OPTICAL ANISOTROPY IN (311) $\text{In}_{1-x}\text{Ga}_x\text{As}/\text{GaAs}$ QUANTUM WELLS

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Quantum wells and superlattices grown on (311)GaAs substrates have become popular owing to the possibility of obtaining lateral confinement through the spontaneous formation of quantum wires during growth. In AlGaAs/GaAs (311) superlattices, lateral confinement was diagnosed by the appearance of optical anisotropy in the reflectivity and absorption spectra. We define an anisotropy parameter γ , which depends on the ratio, R , of the intensities between the heavy and light-hole transitions for polarizations along and perpendicular to the growth axis. This parameter, $\gamma = 1 - \frac{R(0\bar{1}1)}{R(233)}$ with $R = \frac{I(hh)}{I(h)}$, is identically zero for bulk materials or for substrates with a high symmetry axis such as (100). On the other hand, the type of corrugation that leads to quantum wires produces lateral confinement along the $(0\bar{1}1)$ direction leading to positive values of γ , with $\gamma \rightarrow 1$ as the lateral confinement increases. It has been argued that a similar trend could be observed for very thin non-corrugated quantum wells as a result of the 2D-confinement of the intrinsically anisotropic valence bands. Both effects would lead to $\gamma \neq 1$ with γ increasing as the QW-width decreases. In the present work we make a detailed optical study of $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ ($x \simeq 0.2$) strained quantum wells grown by MBE on GaAs substrates with both (100) and (311) orientation. The samples were also studied by double crystal x-ray diffraction in order to characterize the strain contribution and other structural parameters. In these samples three sources of anisotropy are possible: a) the one associated with confinement along the growth direction as a consequence of the anisotropy of the valence band, b) a second one which results from the wave function mixing provoked by the strong bi-axial strain and c) a third one associated with the in-plane component of the piezo-electric field, which is also a consequence of bi-axial strain. Of these causes only the first should depend on the well thickness (d), while the others should be independent of this parameter. Results on samples with $d = 40\text{\AA}$ and $d = 100\text{\AA}$ show $\gamma \simeq -0.87$ and $\gamma \simeq 0.54$ respectively, for the (311) samples. Hence γ seems to be strongly dependent on well-width which favors the mechanism of wave-function mixing due to confinement along the (311) direction.

MODIFIED OBE EQUATIONS

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The concept of a radiative damping (RD), i.e. an intrinsic friction, arises already under *classical* approach to the problem of a matter-field interaction. However, under employment of this generally accepted model in classical molecular optics the RD effects are always disregarded. In Ref¹, RD effects were firstly considered jointly with discrete properties of a medium. Only with allowance of the both of these factors model of frictionless (without RD) classical oscillator acquires a basis for application. The true reason for adoption of such a model consists in exact cancellaion of the RD and discrete effects². On the other hand, under consideration of a *semiclassical* system (two-level atom + classical field) by means of the optical Bloch equations (OBE) no classical relaxation terms whatever enter these equations. They appear only with adaptation of a quantum mechanical treatment. It seems interesting to find out the possibility to account classical RD effect within the same classical frameworks.

What modifications of the OBE must be done to describe the RD effect? The essence of the problem becomes clear if we consider elementary problem of conservation of energy in a process of resonance fluorescence of an isolated dipole \vec{d} under action of a monochromatic field \vec{E} . The total flux of energy through a surface around the dipole is

equal to $\int \vec{s} \cdot \vec{n}_\Sigma d^2 r_\Sigma = \omega \left(\frac{k^2}{3} |\alpha|^2 - \frac{\alpha''}{2} \right) |\vec{E}|^2$, where $\alpha = \alpha' + i\alpha''$ is the polarizability of the dipole. For nondissipative atom this flux must be equal zero, so that $\alpha'' = \frac{2}{3} k^2 |\alpha|^2$.

However, the standard form of OBE requires that α must be purely real. How satisfy these contradicting requirements? The detailed analysis of the OBE in terms of self-consistent field prompts the following natural generalization of OBE due to RD: the

substitution $\vec{E} \rightarrow \vec{E} + \frac{2}{3} \frac{\vec{d}}{c^3}$ must be done. In slow-varying amplitude approximation the additional terms take form $\omega^4 |\vec{d}|^2$ and $\omega^3 \vec{d}$, so that OBE turn into

$$\dot{\vec{d}} + (\Gamma - i\Delta)\vec{d} = -\frac{i}{2} f \frac{e^2}{m\omega} \vec{E}, \quad \dot{N} + \gamma(N - N^*) = \frac{\omega}{h\omega_0} \text{Im}(\vec{E}^* \cdot \vec{d}) - \frac{2}{3} \frac{\omega^4}{3h\omega_0 c^3} |\vec{d}|^2 \quad (1)$$

For Eqs.(1) flux of energy depends only on one relaxation parameter γ and equal to $h\omega_0(W_2 - \gamma N_2)$, where W_2 and N_2 are pumping rate and number of atoms on the upper level, correspondingly. This relation satisfies the conservation energy law automatically.

The developed approach allows to understand the price which one is obliged to pay in order to satisfy law of conservation of energy in the framework of the semiclassical theory. Namely, one compel to assume that some part of the relaxation term γN is connected with the emission of photons of the coherent field \vec{E} and such process don't lead to loss of energy from the system "atom + coherent field".

1. A.V.Ghiner and G.I.Surdutovich, Optics & Photonics News, December, 34 (1994).
2. A.V.Ghiner and G.I.Surdutovich, submitted to Phys.Rev.A.

**SUPERLATTICES IN THE PRESENCE OF EXTERNAL AC
ELECTRIC FIELDS:FREQUENCY COMMENSURABILITY
EFFECTS IN DRESSED MINIBANDS**

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The behaviour of electrons in semiconductor heterostructures, interacting with strong external AC fields, has been a subject of growing interest in the past few years. Recent developments in fabrication of semiconductor microstructures and tunable far-infrared lasers led to a new field of investigation, relating Quantum Optics and Solid State Physics. One of the striking predictions is the collapse of superlattices minibands[1], as well as resonant tunneling suppression[2] for certain intensities of external AC fields. The evolution of dressed electronic states, starting from bare electronic states, gives rise to Brillouin Zones of quasienergies[1]. In the present work we describe an electronic miniband with a tight-binding model. The interaction with a laser field of a given frequency is described by a time-independent Hamiltonian which replaces the semiclassical time-dependent Hamiltonian[3]. The eigenvalues from a field-intensity dependent quasienergies spectrum. We extend the interaction to a simultaneous second strong external AC field. A time independent Hamiltonian can be obtained if the frequencies of both fields are commensurate. We analyze the self-similar properties of the dressed electronic spectra. We also investigate the electronic properties of an isolated quantum dot interacting with external intense AC fields in the presence of a static magnetic field. Modification of Hofstadter-like spectra due to intense AC fields is also addressed

¹ Martin Holthaus and Daniel Hone; Phys. Rev. B **47**, 6499 (1993)

² Mathias Wagner, Phys. Rev. B **49**, 16544 (1994)

³ J. H. Shirley, Phys. Rev. **138**, B979 (1965)

**ELECTROMAGNETIC PROPAGATOR OF A SEMICONDUCTOR
SUPERLATTICE WITH BROKEN TRANSLATIONAL SYMMETRY
IN AN EXTERNAL MAGNETIC FIELD**

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Abstract. We calculate the components of the photon propagator in a superlattice with an electron layer which breaks the translational symmetry of the system. It is shown that in the presence of an external static magnetic field it is possible to excite localized modes of the helicon and magnetoplasma-type in the retarded region of spectra. The conditions for the existence of such modes are discussed and their features are illustrated with the corresponding dispersion curves and power spectra. We also have investigated the influence of a random distribution of defect layers on the dynamics of the electron system. For this purpose we have solved the Dyson's equation for such system in the frame of the T -matrix method in the approximation when the distance between defect layers is much greater than the parameter associated with the localization length of such modes.

**SPLITTING PATTERNS AND SELF-SIMILARITY IN A CLASS OF
ONE - DIMENSIONAL GENERALIZED FIBONACCI SUPERLATTICES**

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We present calculations of the electron energy levels in a one dimensional *Fibonacci* semiconductor superlattice using the transfer - matrix method for electron transmitted through layered $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ at zero field. The structure was created when two different layers $\text{Al}_x\text{Ga}_{1-x}\text{As}$ (A) and GaAs (B) are arranged according to the following recursion relations $A \rightarrow AB$ and $B \rightarrow A$. The energy spectrum has a very special hierarchical and self-similar structure: in every hierarchy, we found that the energy spectrum of the *Fibonacci* lattice has a trifurcating structure. The transmitted wave packet presents clear evidences of fractality reproducing those of the underlying energy spectrum; the dominant effect is the resonant coupling among the states of the same energy. We show that the energy spectrum has a global structure with three subbands where each subband is further splitted into a hierarchy of one up to three subbands.

TRANSITION FROM THREE- TO TWO-DIMENSIONAL MAGNETO-EXCITON

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The optical transitions in direct gap semiconductors are dominated by the excitonic states. These effects are even more pronounced in low-dimensional semiconductors. In the 3-dimensional (3D) limit, the electron and hole are strongly correlated in all directions, forming a 3D-exciton. On the other hand, for a strongly confined quantum well (QW), the carriers kinetics along the growth direction is determined by the barrier potential and a quasi 2-dimensional (2D) description is well suited to describe the excitonic states. An interesting situation arises for large QW widths or shallow QW barriers when the confinement potential and the Coulomb interaction are of the same order (M. Fritze et al., Phys. Rev. Lett. **76**, 106 (1996)).

We present the results of the calculation of the exciton states in these situations for the GaAs-(Ga,Al)As system. A center-of-mass quantization of the 3D exciton is used to describe the effects of the QW barriers. As the quantum well width decreases or depth increases, the breaking of translational invariance leads to a 2D-like exciton. In this case, the exciton wave function undergoes a deformation and the relative motion couples with the center-of-mass motion. We also consider the presence of an external magnetic field applied perpendicular to the growth direction. The magnetic field induces a coupling between the center-of-mass and the relative motions. We study the exciton states focusing on the mixing of the relative and center-of-mass motion for various well widths and intensity of magnetic field, from very shallow to deep quantum wells, to visualize the change of dimensionality of the system.

EFFECTS OF INTERNAL STRAINS ON RESONANT TUNNELING OF HOLES

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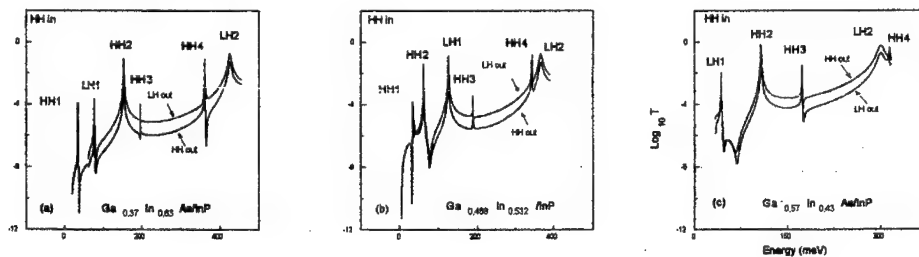
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Considerable interest on resonant tunneling of carriers lies in their direct applications to electronic devices, such as oscillators for example, operating in high frequency regime.

We made an detailed theoretical study of the effects of internal strains on mixing of resonant hole states in double-barrier structures under different strain conditions and external fields. We are able to show how tunneling probabilities and current of holes carriers can be drastically affect by the type of axial strain imposed by lattice mismatch. Figures below are examples of two $\text{Ga}_{1-x}\text{In}_x\text{As-InP}$ (under compression(a) and extension(c)) and one lattice-matched $\text{Ga}_{0.499}\text{In}_{0.501}\text{As-InP}$ (no strain(b)) samples, showing how one could make use of internal strains to improve performance and quality of electronic devices.



POLARONIC EFFECTS ON THE DYNAMICAL PROPERTIES OF A SASER

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A SASER is a new device capable of generating an intense coherent beam of short wavelength phonons which could have a large variety of applications, like three dimensional imaging at nanoscopic scale, phonoelectronic devices, and phonolithography for ultra large scale integrated circuits.

In previous works we studied an elementary model¹, its dynamics² and the polaronic effects on its static properties³.

The device consists in a double barrier heterostructure (DBHS) tailored in such a way that the energy difference between the two lowest resonant levels in the well is near the LO-phonon energy. This LO-phonon decays in a pair of phonons producing a SASER beam.

The system is described by a tight-binding Hamiltonian for the electrons, a single confined mode for the phonon and an electron-phonon interaction. This interaction produces, near the condition for phonon emission, a pair of polaronic states through which the electron can tunnel.

In this paper we have obtained for the polaronic model an analytical solution applicable to the study of the dynamical properties.

The results shows instabilities in a small region of the applied bias, depending on the parameters of the system, meaning that in this region it does not exist a stationary solution for the kinetic equations describing the device. The temporal behavior of these solutions is characterized applying the usual criteria for dynamical systems.

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2. J. Weberszpil et al, *Proceedings of the ICPS 23*, 4, 3299 (1996)
3. D.E. Tuyarot et al, *Superlattices and Microstructures* **20**, 7279 (1996)

ULTRAFAST TIME DYNAMICS OF THE OPTICAL ABSORPTION OF CdTe QUANTUM DOTS IN A GLASS MATRIX

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We study the ultrafast dynamics of the optical absorption of CdTe quantum dots in a glass matrix. We use a pump and probe setup with femtosecond duration laser pulses. The pumping pulse, used to excite carriers in the quantum confined states of the dots, is an optical pulse of ~ 150 fs of duration, centered at 614 nm (2.02 eV). The probe, used to measure the changes in absorption generated by the pump, is a white light continuum (580 - 650 nm) of ~ 30 fs of duration. We use this available spectrum to measure the evolution of the absorption changes, as a function of the delay time between pump and probe pulses, at different spectral regions.

Samples, with dot average radii on the order of $R \approx 35$ Å and size dispersion between 5 to 10 %, were fabricated as described in Refs. [1-2], and have absorption spectra consisting of a peak (usually assigned to the lowest lying transition) near the pump pulse energy (~ 2.0 eV) and shoulders at higher energies (higher optical transitions). Their photoluminescence spectra show only a band which correlates very well with the first absorption ("band edge" luminescence). These data show no broad band luminescence at lower energies (infrared region), so our samples are free of deep traps [1].

The evolution of the absorption is very similar for all the samples studied. It shows a bleaching that has an initial fast exponential decay, with time constants between 1.2 to 2.2 ps, and after that reaches a slow decay plateau at a value of ~ 30 % of the maximum. The fast component that we measure is four to six times greater than previously measured [3] in samples fabricated by a different process [4] that show a prominent luminescence band at energies below the band gap (infrared). This corroborate the assignment of these luminescence bands to deep traps and tell us that they must have a predominant role in the decay process. We conclude that the deep traps have a fundamental influence on the recovery rate of these quantum dots.

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TIME DEPENDENT HOT ELECTRON INDUCED DEGRADATION OF MOS CAPACITORS

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The effects of charge carrier injection on the interface degradation in Metal/SiO₂/Si (MOS) structures have been extensively studied¹⁻³ in the past, and for many years have been a problem of great concern towards the making of more reliable devices. Of particular interest is the generation of the interface traps at the SiO₂/Si interface^{2,3}, which are known to affect the electronic properties of transistors and advanced MOS devices used in digital circuitry. A better understanding of the long term behavior of MOS devices under charge carrier injection will contribute to the development of newer advanced MOS technologies.

The devices investigated in this work were fabricated on p-type Si (100) wafers with a resistivity of 10 Ω -cm using a procedure similar to the one as described elsewhere⁸. Fowler-Nordheim electron injection technique^{3,9} was used mainly as a tool for generation of interface traps. A HP Semiconductor Parameter Analyzer 4145B was used in conjunction with a Capacitance x Voltage (C-V) station in order to inject electrons into the oxide, either from the Al-gate or from the Si/SiO₂ interface. The setup allowed for injection to be performed at different levels of constant current or constant voltage. The interface trap distributions of the samples before and after injection were analysed by measuring the high-frequency and quasi-static capacitance-voltage curves.

This work presents results for the interface traps generated by hot electron injection and compares its behavior with those generated in MOS devices damaged by ionizing radiation⁴⁻⁶. More specifically, the qualitative features of the energy distribution of the interface traps, their post-injection time dependence behavior, and their dependence on the gate bias during injection. Most of these, present qualitative characteristics, which resembles the traps generated by ionizing radiation.

The Fowler-Nordheim electron injection experiments in MOS capacitors, however, has indicated that the interface trap generation process and behavior is quite different when the hot electrons are injected either from the silicon substrate side or from the metal-gate side. The interface traps dynamically change its distribution in the band gap with time after the electron fluence is ceased, but a two-peaked interface trap distribution is present only if injection is performed from the silicon substrate. In addition to the interface traps generated immediately after hot electron injection, we have studied its long term time dependent behavior as a function of electron fluence from the gate or from the substrate side of the MOS capacitors. The rate of change in time of the interface traps has been found to be a function of the gate-induced strain and the magnitude of the initial damage level. These, in turn, affect the long term time dependence as a function of current density, electron fluence, device area, and the gate bias polarity during injection.

These findings suggest the possibility of using the results from the hot electron experiments to predict the behavior of the interface traps after exposure to ionizing radiation, and vice-versa. The practical significance relies on the fact that more flexibility is obtained for designing experiments to test either the radiation response or the hot electron response of MOS structures. For certain device structures (e.g., devices already packaged with significant shielding) it may not be practical or convenient to study their radiation effects; in this case one will be able to obtain a good idea of their radiation responses by performing the hot electron experiments.

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QUANTUM SIZE EFFECTS IN ONE-DIMENSIONAL DISORDERED QUANTUM WELLS

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Disordered one dimensional systems, exhibiting nontrivial extend states have been a subject of great interest in the past few years. One dimensional finite systems showing clear mobility edges open a useful scenario to understand some fundamental questions related to the existence or not of quantum confinement in strongly disordered heterostructures, like quantum wells made of amorphous semiconductors. The research efforts devoted to heterostructures based on amorphous semiconductors have not yet established a clear picture of the related quantum size effects in this context. Here we study the electronic structure of quantum wells, where the well material is a repulsive binary alloy, described by a tight-binding model. We find bona fide confined states in the energy range where the bulk material presents states with a localization length at least three times longer than the quantum well width. These results due to the competition between localization length and quantum size effects, are also verified in the transmission probability of these double barrier structures. Some clear transmission resonances related to bona fide quasi-bond states are identified. These bona fide quantized states show clear parity properties in spite of the disorder. We also extended the model to analyze coupled quantum wells under an external electric field and the formation or not of minibands in finite disordered superlattices.

SPECIFIC HEAT IN DOPED QUANTUM WELLS, THE SCHOTTKY ANOMALY.

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During the growth process of semiconductor hetero-structures there are, intentionally or not, the presence of impurities. For a doped and partially compensated quantum well, with shallow donors as majority impurities and at low temperatures, it is observed neutral and ionized donors and ionized acceptors. Baranovskii et al calculated the thermal properties of compensated bulk semiconductors by the Monte Carlo method. They simulated the distribution and occupation of impurities through random numbers. For each impurity distribution the donor occupation numbers change as temperature increases, due to transitions of electrons between donors. Finally it is taken an average over a large number of distributions.

We treat a compensated quantum well using a self-consistent method. Starting from a suitable electric charge density, homogeneous in the direction normal to the growth axis, we calculate the electrostatic potential, the corrected energy of electrons bound to donors and the density of states of the system. Assuming the neutrality of the electric charges we obtain the electronic chemical potential and we recalculate the charge density. This procedure is repeated until the convergence of the chemical potential is reached for a range of temperatures.

The specific heat obtained presents the Schottky anomaly due to the limited value of the energy of the system. This effect is characterized by a maximum in the specific heat and may be used to diagnose the impurity concentration and compensation of the quantum well. For a GaAs-GaAlAs quantum well, with donor concentration of 10^{10} cm^{-2} , the maximum occurs at temperatures close to 10 K, varying very little with the compensation but showing a sensible difference on the intensity of the specific heat.

Another interesting effect is the dependence of the chemical potential with temperature, showing an extremum (minimum for low compensation and maximum for high compensation) due to the form of the density of states.

**STUDY OF RADIATIVE RECOMBINATION PROCESSES IN $\text{In}_x\text{Ga}_{1-x}\text{As}$
QUANTUM WELLS GROWN ON GaAs (100) MISORIENTED SUBSTRATE**

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The strained $\text{In}_x\text{Ga}_{1-x}\text{As}$ quantum well has recently received considerable interest for optoelectronic device applications due to the small electron effective mass, high electron mobility at room temperature and possibility for band gap engineering in a wide range. Strained InGaAs layers on slightly misoriented substrate were actually grown by various epitaxial growth methods including molecular beam epitaxy (MBE). The advantages for using misoriented substrates include superior optical, surface and interface quality of the epilayer. In order to better understand these improvements, we have grown by MBE high quality $\text{In}_x\text{Ga}_{1-x}\text{As}$ quantum wells (QW) with indium concentration of 15% on misoriented substrate (2° , 4° e 6° off) towards the direction $[111]\text{A}$, with well width of 100\AA . The samples were grown by MBE in our laboratory and studied with respect to their optical properties. A nominal (0° off) sample was also grown as a reference. In low temperature (2K) photoluminescence (PL) measurements, a significant blue shift of the PL energy peak with a simultaneous decreasing on the PL linewidth was observed when going from nominal to 6° off. This behavior is a consequence of the change of the intrinsic ground state excitonic transition energies. It can be explained in terms of a regular shrinkage of the well width due to terrace edges, additional stress of the well material at the step edge, and an orientation dependent In segregation. In order to study the carrier escape phenomenon from the well, we have performed temperature dependent PL measurements on the samples. At low temperature, we observe that the PL intensity, of the emission associated to the quantum well grown on slightly misoriented (100) GaAs substrate, exhibits a larger intensity as compared to a QW grown on perfectly oriented substrate. At high temperature, the PL intensity of both wells (misoriented and nominal) becomes identical. The observed temperature dependence of the PL intensity is modeled in terms of thermally activated escape of electron-hole pairs from the well. We find that this model fits the data for low ($T < 40\text{K}$) and high ($T > 80\text{K}$) temperature. For intermediate temperatures we have to consider another nonradiative recombination process, being, the escape of the less-confined carrier species from the QW. With this treatment we are able to deduce the activation energy for the electron-hole pair escape from the QW as well as for the holes (less confined carrier). Different values for nominal and misoriented samples are observed.

CRITICAL ANALYSIS OF THE VIRTUAL CRYSTAL APPROXIMATION*

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We investigate the validity and limitations of the Virtual Crystal Approximation (VCA), widely and successfully adopted to describe random semiconductor alloys. Two simple problems are studied in this context.

First we consider a single quantum well of GaAs, with width W , confined by $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ barriers. The energy of the first electronic state (E_{C1}) is calculated through the envelope function approximation (EFA), which involves the effective mass approximation and the VCA in the alloy region. Results for E_{C1} thus obtained are compared to the values determined within the tight-binding approximation using a sp^3s^* parametrization for the different atomic species, which allows a realistic treatment of the alloy disorder effects. For well widths W above 80 Å, a good agreement is obtained for $E_{C1}(W)$ in both calculations. For narrower wells the tight-binding results are consistently lower in energy, differing by as much as 100 meV for wells only a few monolayers thick. Performing tight-binding calculations with the alloy region treated in the VCA, the agreement with the EFA increases to cover essentially the whole range of W values. We therefore conclude that the main limitation of the EFA in the treatment of narrow wells comes from the VCA. Results for the wave functions and superlattices bandwidths will also be presented.

The second problem considered regards bulk $\text{Al}_x\text{Ga}_{1-x}\text{As}$ alloys. We perform a spectral decomposition of the main gap wave functions determined through tight-binding supercell calculations. The amount of zinc-blende symmetry character in the wave functions of direct and indirect gap structures is investigated and compared to the VCA predictions.

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THE INFLUENCE OF HYDROSTATIC PRESSURE ON THE LINE SHAPE OF EXCITONIC RECOMBINATION IN (311)A QUANTUM WELL

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It has been recognized that a deconvolution of experimental line shapes might provide quantitative information on structural properties¹ of the two interfaces of a quantum well (QW) or on impurity incorporation^{2,3} at the growth surface. Excitons in this case are ideal sensors of atomic scale because they can probe the influence of interface structure on the optical properties. We have used the hydrostatic pressure as a tool to change the exciton environment which in turn leads to changes in the QW photoluminescence line shape and intensity. The linewidth variation on pressure is analyzed on the basis of size interface fluctuations⁴. It was also observed that the line shape at 300K for a (311)A oriented QW changes from Lorentzian to Gaussian broadening by increasing the laser power at different pressures. It is well known that the magnetic field applied along the growth direction affects the size of the exciton. This fact turns out the magnetic field another powerful tool to probe the QW interface structure. The dependence on magnetic field affected directly the linewidth and have enabled us to obtain information concerning the microscopic details of our QW interfaces.

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ELECTRIC FIELD INDUCE DELOCALIZATION IN AN APERIODIC SEMICONDUCTOR HETEROSTRUCTURE.

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One of the fundamental properties of a periodic heterostructures that makes it useful in electronic and optical applications is the nature of electronic states, i.e., the wave function extended over entire system with the formation of mini-bands analog as formed in bulk materials. The mini-band width depends of the coupling degree between the eigen-states related to the system parameters such as: barrier thickness, effective mass and the applied external field. The application of an external field in a periodic system leads to a host of interesting effects related to the transition between extended to localized quantum states of the system. By the application of the field along the growth axis the mini-bands breaks under the field in to a Stark-ladder of states whose wave functions gradually lose the extended behavior.

In this work, we observed a contrary effect of an external field when applied in an aperiodic semiconductor heterostructure, i.e., the field induce delocalization in the electronic states and a mini-band formation. Using the Split-Operator method we simulated an aperiodic finite heterostructure which consist in a sequence of alternating layers of GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ($0.1 \leq x \leq 1$) whose the thickness of wells and barriers increase gradually in the structure. The symmetry breaking at zero applied external field induce a localization of the electronic wave functions, increasing the coupling and the system properties becomes to a superlattice regime near a electric field value (which depends on the parameters of the system). At this field, the mini-band width have the minimum value and the Bloch like oscillations have the maximum amplitude. This system open the possibility to obtain a new conception of design in semiconductor devices possible applied to optical-modulators extremely sensitive to low external fields.

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CLASSICAL MODEL OF CLUSTERS OF SCREENED CHARGES IN QUANTUM DOTS

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Recently there has been an explosion of interest in the theoretical study of the two-dimensional (2D) system of charged particles confined by a external parabolic potential. This system have been used as models of radio-frequency traps for ions and electrons in plasma, heavy-ion storage rings, and electrons in bubbles above liquid helium and in semiconductor quantum dots. Previous studies are based on Monte Carlo simulations in which artificial atomic-like behavior of the confined cluster of particles have been reported.

In this work, we consider a more realistic model for quantum dots by taking into account the screened interaction between the particles confined in a parabolic well. Molecular Dynamics simulations were performed to investigate structural and dynamical properties as a function of the screening parameter for different cluster sizes. We obtain an interesting new structural phase-transition from configurations of rings to the Wigner crystal and the phase-diagram is analyzed.

HOLE BAND STRUCTURE OF Si-BASED p -TYPE δ -DOPING QUANTUM WELLS

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δ -doping is a powerful method to create confined carrier gases of relatively high concentrations and mobilities. In GaAs and Si, both n - and p -type δ -doping structures have been grown successfully by means of Molecular Beam Epitaxy. While the energy band structures of the confined electron and hole gases in GaAs, and that of the confined multi-valley electron gas in Si, are well-known from self-consistent envelope function calculations, the hole band structure of p -type δ -doping wells in Si has been investigated only within a simple one-band model thus far [1]. The latter treatment is expected to be even less reliable in the case of Si than in the case of GaAs because, due to the small spin-orbit splitting energy of Si (44 meV), the spin-orbit-split band will be involved in the formation of the confined hole states; in the case of GaAs, this band is far away (340 meV). On the other hand, the spin-orbit splitting energy in Si is not small enough to be neglected with respect to the confinement energy. In this regard, the theory of the hole band structure of p -type δ -doping wells in Si faces an 'intermediate' case which is always more difficult to solve than limiting cases. The proper way of including the spin-orbit-split band is to employ the 6×6 Luttinger-Kohn Hamiltonian. The corresponding 6×6 multiband envelope function equation forms the basis of our calculations. It is represented with respect to a basis set of plane waves. Hole-hole interactions, including exchange and correlation, are taken into account in self-consistent way. The method is used to calculate potential profiles, subband and miniband structures as well as Fermi level positions for a series of p -type δ -doping quantum wells. The hole wells turn out to be relatively flat in comparison with electron wells in the case of n -type δ -doping. This is similar to GaAs, and is mainly due to the strong localization of heavy holes and the pertinent effective screening of the ionized acceptor sheet. We find that sheet doping concentrations larger than 10^{12} cm^{-2} are necessary for confinement effects to be observable. This is in agreement with experimental photoluminescence results [2] performed on p -type δ -doping structures with doping concentrations in the range from 10^{12} cm^{-2} to 10^{14} cm^{-2} .

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Low Angle X-Ray Reflection Studies of InGaAs/InP Multiple Quantum Wells

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Abstract : Low angle x-ray reflectometry was applied to an InGaAs/InP multiple quantum well structure containing 20 periods in addition to a cap and a buffer InP layers. A dynamical simulation, using the multireflexion phenomena and absorption, was employed to determine the thickness of the different layers. The thickness of the InGaAs quantum wells and of the InP barriers were determined to be 30 Å and 92 Å, respectively, with a 1 Å precision. Also, the cap layer thickness was evaluated to be (200 ± 5) Å, being the first layer thickness determination in a asymmetrical layer structure. Results obtained by photoluminescence and high angle x-ray diffraction are compared and discussed, confirming our results. Information about interface roughness is extracted from the comparison between experimental and simulated data, as well, indicating a non detectable roughness level.

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a) On leave from A. F. Ioffe Physico-Technical Institute, Saint - Petersburg, Russia.

DONOR CONCENTRATION EFFECTS ON THE POTENTIAL PROFILE OF QUANTUM DOTS[†]

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Within the framework of effective mass theory, we have determined the radial potential profile of the Reed's type quantum dot. The Poisson's equation with charge density given by Thomas-Fermi approximation were solved numerically and self-consistently. Our results show that the anharmonicity of radial potential increases with donors concentration at contact region.

On the other hand, the behavior of radial potential inside the dot is almost perfectly parabolic. This behavior is broken only at region very close to the lateral surface. Probably, this deviation is important only if a very high applied bias is involved in the measurement of tunneling current.

Finally, band bending near epitaxially constructed barriers were studied. The inversion layer increases near longitudinal barrier with the concentration of donors.

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FINITE SIZE EFFECTS ON ANTIDOTS ARRAYS IN MAGNETIC FIELDS

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New short-period lateral superlattices envisage the possibility of observing the manifestation of Hofstadter-like spectra in magnetotransport measurements. The observability of such effects raises questions about the lower limit for the size of a finite lateral superlattice in order to define self-similar signatures in the electronic structure of the system. We show in the framework of a tight-binding model that these signatures are already present in small systems, which one could call "lateral molecules".

On the other hand, the coupling of bulk and edge states can be tuned by magnetic field, as well as by independent electrostatic modulation of the "bulk" and "surface" of the system. This flexibility could be used to distinguish the two types of edge states we predict for the finite lateral superlattice: *i*) bona fide edge states confined to the surface with tunable coupling to the bulk, and *ii*) edge states in the internal structure of the bulk self-similar spectra. The tight-binding model is also extended for lateral superlattices in the presence of a modulated magnetic field.

THE STRUCTURE OF Si/Ge SUPERLATTICES

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Heterostructures based on Si and Ge, deposited on (100) silicon single crystalline substrates by Molecular Beam Epitaxy (MBE), were analyzed by means of x-ray diffraction techniques. The MBE deposition method allows the growth of monolayers in atomic scale with composition control, provided a precise adjustment of the deposition parameters. Nevertheless, it is demanding to verify the real obtained structure, which requires sample's characterization after the deposition procedure. Among the non-intrusive characterization methods, x-ray diffraction has been used currently. The conventional rocking-curves give the relevant structural parameters: superlattice mean period, perpendicular and in-plane lattice parameters, structural strain and interface properties. In this work, different Si/Ge heterostructures were analyzed, which consisted of a superposition of two structures: (i) an internal one with a period d , formed by Si-Ge bilayers, and (ii) another with a larger periodicity D , formed by six of the former Si-Ge bilayers spaced by a Si buffer layer, whose function is to decrease the stress due to the difference in Si and Ge lattice parameters. The whole system is repeated ten times. The thickness of the Si-Ge structure varies from 5 to 7 monolayers, while the Si spacer is around 360 monolayers. The x-ray diffraction characterization were performed in two different setups: powder diffractometer (θ - 2θ geometry) and double crystal diffractometer (rocking-curve). Monochromatic Cu K α radiation was used in the angular region of $2\theta \approx 1^\circ - 80^\circ$. The determination of the structural parameters was based on the higher intensity measurements obtained with the powder diffractometer and on the higher resolution data collected with the double crystal setup. The experimental results were computer simulated by means of kinematical and dynamical x-ray diffraction theories, whose results were compared and discussed. The structural parameters were obtained by at least two independent experimental data and compared with the nominal values.

**Projeto for the Installation of an
Electron Microscopy Center
at the LNLS**

TU-71

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The development of modern technology cannot be carried out without a well established materials science know-how. From a more basic point of view, the association of chemical composition and atomic structure with the macroscopic physical and chemical properties of materials requires the use of a wide variety of characterization techniques. Among the most popular structural tools for bulk samples, we may mention X-ray diffraction, X-ray absorption spectroscopy, phototemission, etc. Most of these experiments provide excellent quality data but averaged over a large area/volume of the sample, usually in the millimeter range (advancing to the sub-millimeter range in high brilliance synchrotron light sources). The manipulation of matter in the nanometer and sub-nanometer range has become standard procedure, and at present, high spatial resolution (< nanometer range) is required for the characterization of most modern synthetic materials of which semiconductors heterostructures, magnetic multilayers, porous silicon, etc. are well-known examples. Both approaches, spatial resolution and spatially averaged information are complementary and cannot be ruled out for modern competitive science and technology.

We propose to create a center for electron microscopy (transmission and scanning) specially oriented to high resolution (of the order of nanometers) studies. These techniques constitute one the basic tools of modern research in chemistry and physics of solids and although the research of several groups deals with nanostructured materials, these techniques are at present lacking in Brazil. The high resolution electron microscopy facility is being suggested to fill this gap within the shortest possible delay, so that Brazilian scientists will be able to perform their work in a highly competitive and stimulating situation, when compared to developed countries. The center will be organized as a multi-user open facility attached to the National Laboratory for Synchrotron Light, so that the scientific and technological communities will have access and be able to profit from its capabilities. At present, several proposals have been submitted to funding agencies (state/federal) in order to get funds for the acquisition of the electron microscopes and sample preparation laboratory.

CORRELATION EFFECTS OF DX CENTERS ON ELECTRON MOBILITY IN DELTA DOPED GaAs BY MONTE CARLO SIMULATIONS

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We present a theoretical study of correlation effects of charged impurities on electronic properties of highly (Si) δ -doped GaAs. In such a system several electronic subbands are populated, and at low temperature ionized impurity scattering is the most important scattering mechanism. Increasing doping density and/or applying a hydrostatic pressure increases the population of the DX state, which is helpful to show these correlation effects in the system.

Much experimental work has been done on δ -doped semiconductors in the presence of external pressure in order to observe the effects due to DX centers. However, only a few number of theoretical studies have included spatial correlations in their calculation. Using the widely accepted d^+/DX^- model, we have described the measured results deduced from Shubnikov-de Haas measurement by Skuras *et al.* [1] for the population and the quantum mobility of electrons in different subbands. A reasonable agreement between theory and experiment is reached for pressures not in excess of 10 kbar.

By approximating the pair correlation functions of the charge distribution in two dimensions by step functions, the equilibrium equation of the reservoirs of filled DX centers and the quasi-two-dimensional electron gas are solved self-consistently. This gives the electron density of the subbands which were found to be in excellent agreement with the experimental findings [1]. The DX energy and its derivative with respect to pressure were determined to be 290 meV and -9 meV/kbar, respectively, which are consistent with the values reported in literature [2].

The influence of the correlations of the charged impurities on the electron mobility is taken into account by the structure factor of the charge distribution in the δ -layer. This factor is determined by the Fourier transformation of the pair correlation functions. By comparing the measured quantum mobility [1] to theoretical results obtained with three different methods: (1) no correlation effects [3], (2) in the step-function approximation, and (3) Monte Carlo simulations of the charge distribution, we have found that the theoretical analysis underestimates the electron mobility systematically in the models (1) and (2), while model (3) gives an excellent agreement for the lowest subband, and a qualitative behavior but twice as large as the experimental data for the excited subbands.

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FAST RISETIME REVERSE BIAS PULSE FAILURES IN SiC PN JUNCTION DIODES

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SiC based high temperature power devices are being developed for aerospace systems which require high reliability. To date it has necessarily been assumed that the breakdown behavior of SiC PN junction will be similar to highly reliable silicon based pn junctions. Challenging this assumption we report the observation of anomalous unreliable reverse breakdown behavior in moderately doped ($2\text{--}3^{17}\text{ cm}^{-3}$) small and 4H and 6H-SiC junction diodes at temperatures ranging from 298K to 873K. We propose a mechanism in which carrier emission from unionized dopants and/or deep level defects lead to this unstable behavior.

TRANSITION BETWEEN HEAVY HOLE - LIGHT HOLE STATES IN THE VALENCE BAND OF CdTe AT TEMPERATURES 5K - 350K

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Cadmium telluride is still attracting great interest because of its applications as the substrate material in CdHgTe optoelectronic devices, as detectors used in studies of nuclear reactions, and in solar cell technology. The greatest difficulty encountered in the use of cadmium telluride in the fabrication of substrates is a high density of defects such as dislocations, which has an undesirable effect on optical and electrophysical characteristics of epitaxial films grown on semiinsulating substrates.

It was found that in a wide temperature range between 5K and 350K the absorption spectra of cadmium telluride crossed at one point in the infrared range of wave numbers at about 1500 cm^{-1} (0.186 eV). This effect was accounted for satisfactorily by considering intersubband transitions and allowing for corrugations at the top of the valence band.

We investigated *p*-type CdTe single crystals grown by the modified Bridgman method and characterised by room-temperature values of the electrical resistivity $(0.5\text{--}2.5)\times 10^2\text{ }\Omega\cdot\text{cm}$ and carrier mobility $40\text{--}80\text{ cm}^2\text{V}^{-1}\text{s}^{-1}$. At $T=300\text{K}$ the carrier density was $10^{15}\text{--}10^{18}\text{ cm}^{-3}$.

The optical spectra were recorded using a Bruker IFS-113v Fourier transform spectrometer.

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